



Analysis of some heterogeneous catalysis models with fast sorption and fast surface chemistry

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Dedicated to Matthias Hieber on the occasion of his 60th birthday

Abstract. We investigate limit models resulting from a dimensional analysis of quite general heterogeneous catalysis models with fast sorption (i.e. exchange of mass between the bulk phase and the catalytic surface of a reactor) and fast surface chemistry for a prototypical chemical reactor. For the resulting reaction–diffusion systems with linear boundary conditions on the normal mass fluxes, but at the same time nonlinear boundary conditions on the concentrations itself, we provide analytic properties such as local-in-time well-posedness, positivity, a priori bounds and comment on steps towards global existence of strong solutions in the class $W_p^{(1,2)}(J \times \Omega; \mathbb{R}^N)$, and of classical solutions in the Hölder class $C^{(1+\alpha, 2+2\alpha)}(\bar{J} \times \bar{\Omega}; \mathbb{R}^N)$. Exploiting that the model is based on thermodynamic principles, we further show a priori bounds related to mass conservation and the entropy principle.

1. Introduction

In chemical engineering, catalytic processes often play an important, if not predominant role: Certain chemical reactions taking place within a chemical reactor are supposed to be accelerated, whereas other, usually undesirable, side reactions should be suppressed. This aim can be accomplished by adding substances which catalytically act in the fluid mixture (homogeneous catalysis), or e.g. by using suitable coatings for the reactor surface (active surface) which may then act as a catalytic surface to accelerate the desirable reactions on the surface. In many cases, such heterogeneous catalysis mechanisms are actually more efficient by several orders of magnitude than homogeneous catalysts, and, moreover, one may often avoid the need for filtration technology to separate the desired product from the catalyst. Heterogeneous catalysis mechanisms and sorption processes may be modelled starting from a continuum thermodynamic viewpoint by reaction–diffusion systems in the chemical reactor and on the active surface which are coupled via sorption processes, i.e. the exchange of mass between the boundary layer of the bulk phase and the active surface, cf. [20]. In

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accord with their purpose, catalytic accelerated chemical reactions on the surface are very fast, i.e. both the surface chemistry (at least for the desired reactions) as well as sorption processes take place on very small time scales. Hence, it is natural to consider limit models, for which the surface chemistry and sorption are taken to be infinitely fast, i.e. surface chemistry and sorption processes are modelled as if they would attain an equilibrium configuration instantaneously. Using a dimensionless formulation of such coupled reaction–diffusion–sorption bulk–surface systems, several of such limit models have been proposed in [5], including a general formulation of such a fast sorption and fast surface chemistry model. The mathematical analysis of such systems has been accomplished for the case of a three-component system with chemical reactions of type $A_1^\Sigma + A_2^\Sigma \rightleftharpoons A_3^\Sigma$ on the surface, neglecting any bulk chemistry (the latter being no severe obstacle, and for the construction of (uniquely determined) strong solutions not a highly relevant assumption). In the present manuscript, the mathematical analysis is continued for limit systems of the same structure, but for general bulk and surface chemistry. In particular, the results on local-in-time existence of strong solutions, positivity, first blow-up criteria as well as a priori estimates for the solutions will be extended to the generic case.

The paper is organised as follows: In Sect. 2 some basic notation is introduced and some preliminary results are recalled. Thereafter, in Sect. 3, the class of heterogeneous catalysis models considered in this manuscript is introduced and the underlying modelling assumptions recalled from the article [5]. Section 4 constitutes the core of this article and is split into subsections on L_p -maximal regularity of a linearised version of the fast-sorption-fast-surface-chemistry model, on local-in-time existence of strong $W_p^{(1,2)}$ -solutions and classical solutions in the Hölder class $C^{(1,2)\cdot(1+\alpha)}$, on an abstract blow-up criterion as well as a priori bounds, e.g. entropy estimates, on the solution. There is a vast amount of literature on reaction–diffusion-systems or general parabolic systems in the bulk phase with homogeneous or inhomogeneous, linear or nonlinear boundary conditions, e.g. [14, 17] for a start, and quite recently *thermodynamic principles* have become a resourceful driving force for *entropy methods*, e.g. [11–13]. Astonishingly, however, up to now (at least to our knowledge) combined type boundary conditions, i.e. systems where at a fixed boundary point $z \in \partial\Omega$ Dirichlet type boundary conditions are imposed on some of the variables (or, a linear combination thereof), whereas the remaining variables satisfy Neumann type boundary conditions, have only been considered rarely in the literature, see, for example, [14, Chapter 7, Section 10] and the references given therein. Instead, so far most authors focussed on other types of generalisations: for example, in [1, 16, 21] parabolic systems with nonlinear boundary conditions have been considered, but these were always assumed to be of a common order, cf., for example, the *non-tangentiality condition* in [16]. In, for example, [6, 10, 19], general parabolic systems or reaction–diffusion-systems with dynamic boundary conditions have been considered, i.e. typically two parabolic systems in the bulk phase and on the surface are coupled. In [9], on the other

hand, the authors consider more general structures leading to parabolic systems based on the notion of a *Newton polygon*.

2. Notation and preliminaries

Throughout, all Banach spaces appearing are Banach spaces over \mathbb{F} , the field of real numbers \mathbb{R} or complex numbers \mathbb{C} , and $|z|$ denotes the modulus of a real or complex number z , $\Re z$ its real and $\Im z$ its imaginary part. Real or complex vectors (or, vector fields) $\mathbf{v} = (v_1, \dots, v_N)^T \in \mathbb{F}^N$ will be typically denoted by small, Roman letters in boldface and have Euclidean norm $|\mathbf{v}| = \sqrt{\sum_{i=1}^N |v_i|^2}$, whereas matrices $\mathbf{M} = [m_{ij}]_{i,j} \in \mathbb{R}^{n \times m}$ (or $\mathbb{C}^{n \times m}$) most of the time are written in Roman capitals and boldface. The set of natural numbers or integers are denoted by $\mathbb{N} = \{1, 2, \dots\}$ (or $\mathbb{N}_0 = \{0, 1, 2, \dots\}$) and $\mathbb{Z} = \{\dots, -1, 0, 1, \dots\}$, respectively, and vectors of integers $\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_N)^T \in \mathbb{Z}^N$ by small Greek letters in boldface, and with length $|\boldsymbol{\alpha}| = \sum_{i=1}^N |\alpha_i|$, but $\mathbf{v} = [v_{i,j}]_{i,j} \in \mathbb{Z}^{N \times M}$ may also denote integer-valued matrices.

$\Omega \subseteq \mathbb{R}^n$ typically denotes an open and nonempty subset of \mathbb{R}^n , $\overline{\Omega}$ its closure, $\partial\Omega$ its boundary, and $J \subseteq \mathbb{R}$ an interval. Function spaces that are frequently used are $C(\Omega)$ and $C(\overline{\Omega})$ (continuous functions on Ω and $\overline{\Omega}$, resp.), $C^k(\Omega)$ and $C^k(\overline{\Omega})$ ($k \in \mathbb{N}_0$ times continuous differentiable functions on Ω and $\overline{\Omega}$, resp.), $C^{k+\gamma}(\overline{\Omega})$ ($k \in \mathbb{N}_0$ times continuously differentiable functions with bounded and $\gamma \in (0, 1]$ Hölder continuous derivatives of order k), $L_p(\Omega)$ (Lebesgue spaces of order $p \in [1, \infty]$, where as usual function classes are identified with its representatives), $W_p^k(\Omega)$ (Sobolev spaces of differentiability order $k \in \mathbb{N}_0$ and integrability order $p \in [1, \infty)$), $W_p^s(\Omega)$ (Sobolev–Slobodetskii spaces, $s \in \mathbb{R}_+$, $p \in [1, \infty)$). Similarly, one also has their corresponding boundary (for sufficiently regular boundary), Banach space E -valued and anisotropic versions, e.g. $L_p(\Omega; E)$ (E -valued Lebesgue spaces), $L_p(\partial\Omega)$ (Lebesgue spaces w.r.t. surface measure) and

$$C^{(1,2m)\cdot\alpha}(\overline{J} \times \overline{\Omega}) = C^\alpha(\overline{J}; C^0(\overline{\Omega})) \cap L^\infty(\overline{J}; C^{2m\alpha}(\overline{\Omega})), \quad m \in \mathbb{N}, \quad \alpha \in \mathbb{R}_+,$$

$$W_p^{(1,2m)\cdot s}(J \times \Omega) = W_p^s(J; L_p(\Omega)) \cap L_p(J; W_p^{2ms}(\Omega)), \quad m \in \mathbb{N}, \quad s \in \mathbb{R}_+$$

etc.

Remark 2.1. (Sobolev–Slobodetskii spaces and Besov spaces) Recall that for sufficiently regular domains $\Omega \subseteq \mathbb{R}^n$, one has $B_{pp}^s(\Omega) = W_p^s(\Omega)$ for $s \in \mathbb{R}_+ \setminus \mathbb{N}_0$, but $B_{pp}^k(\Omega) \neq W_p^k(\Omega)$ for $k \in \mathbb{N}$ and $p \neq 2$.

For the definitions, basic properties and more information on these spaces, the interested reader is referred to the literature, e.g. [2, 3, 15].

3. The model

In this paper, the following, rather general fast sorption and fast surface chemistry limit model will be considered:

$$\begin{cases} \partial_t \mathbf{c} + \operatorname{div} \mathbf{J} = \mathbf{r}(\mathbf{c}) & \text{in } (0, \infty) \times \Omega, \\ \langle \mathbf{e}^k, \mathbf{J} \cdot \mathbf{n} \rangle = 0 & \text{on } (0, \infty) \times \Sigma, \quad k = 1, \dots, N - m^\Sigma =: n^\Sigma, \\ \exp(\langle \mathbf{v}^{\Sigma,a}, \boldsymbol{\mu}^{\Sigma,a} \rangle) = 1 & \text{on } (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \end{cases} \tag{GFLM}$$

where the appearing variables and coefficients have the following physical interpretation and relations with each other.

Thermodynamic and geometric variables and vectors:

- $\mathbf{c} = (c_1, \dots, c_N)^\top : \mathbb{R} \times \overline{\Omega} \rightarrow \mathbb{R}^N$ denotes the vector field of *molar concentrations*, i.e. $c_i(t, \mathbf{z}) \in \mathbb{R}$ is the molar concentration of the chemical substance A_i at time $t \in \mathbb{R}$ in position $\mathbf{z} \in \overline{\Omega}$, for $i = 1, \dots, N$;
- $\mathbf{J} = [\mathbf{j}_1 \cdots \mathbf{j}_N] : \mathbb{R} \times \overline{\Omega} \rightarrow \mathbb{R}^{n \times N}$ for $\mathbf{j}_i : \mathbb{R} \times \overline{\Omega} \rightarrow \mathbb{R}^n$ the vector field of *individual mass fluxes* of species A_i , $i = 1, \dots, N$;
- $\mathbf{n} : \partial\Omega \rightarrow \mathbb{R}^n$, the *outer normal vector field* to Ω on $\partial\Omega$;
- $\mathbf{r}(\mathbf{c}) = \sum_{a=1}^m R_a(\mathbf{c}) \mathbf{v}^a$, the vector field of *total molar reaction rates* in the bulk phase, modelling chemical reactions given by the formal (reversible) chemical reaction equations

$$\sum_{i=1}^N \alpha_i^a A_i \rightleftharpoons \sum_{i=1}^N \beta_i^a A_i, \quad a = 1, \dots, m,$$

where $\boldsymbol{\alpha}^a = (\alpha_1^a, \dots, \alpha_N^a)^\top$, $\boldsymbol{\beta}^a = (\beta_1^a, \dots, \beta_N^a)^\top \in \mathbb{N}_0^N$ and the *stoichiometric vector* of the a -th reaction is given by $\mathbf{v}^a = \boldsymbol{\beta}^a - \boldsymbol{\alpha}^a \in \mathbb{Z}^N$. Moreover, $R_a(\mathbf{c})$ denotes the molar reaction rate (forward minus backward rate) for the a -th chemical reaction in the bulk phase;

- $\mathbf{v}^{\Sigma,a} = \boldsymbol{\beta}^{\Sigma,a} - \boldsymbol{\alpha}^{\Sigma,a} \in \mathbb{Z}^N$, $a = 1, \dots, m^\Sigma$, are the stoichiometric vectors of the *surface chemical reactions*

$$\sum_{i=1}^N \alpha_i^{\Sigma,a} A_i^\Sigma \rightleftharpoons \sum_{i=1}^N \beta_i^{\Sigma,a} A_i^\Sigma, \quad a = 1, \dots, m^\Sigma,$$

where $\boldsymbol{\alpha}^{\Sigma,a} = (\alpha_1^{\Sigma,a}, \dots, \alpha_N^{\Sigma,a})^\top$, $\boldsymbol{\beta}^{\Sigma,a} = (\beta_1^{\Sigma,a}, \dots, \beta_N^{\Sigma,a})^\top \in \mathbb{N}_0^N$ and the adsorbed versions A_i^Σ of species A_i .

Modelling assumptions:

- The bulk concentrations are assumed to be very small (compared to a characteristic reference concentration c_{ref} of some solute which is not included in the model, $0 \leq c_i(t, \mathbf{z})/c_{\text{ref}} \ll 1$, *dilute mixture*), and the fluid in the bulk is at rest (the basic problem with vanishing barycentric velocity field which will be considered here) or $\langle \mathbf{v}, \nabla c_i \rangle$, i.e. the inner product between the barycentric velocity field \mathbf{v} and the gradient of individual concentrations, is considered as a perturbation, so that Fickian diffusion,

$$\vec{j}_i = -d_i \nabla c_i \quad \text{with some diffusion coefficients } d_i > 0, \quad i = 1, \dots, N$$

is a reasonable (though, not thermodynamically consistent) model for the diffusive fluxes;

- the chemical potentials μ_i in the bulk phase are modelled as those of an ideal mixture with

$$\mu_i(\mathbf{c}, \vartheta) = \mu_i^0(\vartheta) + R\vartheta \ln x_i, \quad i = 1, \dots, N,$$

where $\mu_i^0(\vartheta)$ corresponds to some temperature-dependent chemical equilibrium and $x_i = \frac{c_i}{c}$ is the scalar field of molar fractions, where $c = \sum_{i=1}^{N+1} c_i$ is the total concentration in the bulk phase, including the concentration of some solvent A_{N+1} . Instead of including the solvent A_{N+1} in the model, we replace c by some constant approximation c_{ref} to the actual total concentration c , so that we may consider the vector $\mathbf{x} = (x_1, \dots, x_N)^\top = c/c_{\text{ref}}$ and its dynamics instead of \mathbf{c} . Formally assuming $c_{\text{ref}} = e^{R\vartheta}$, we then have $\mu_i(\mathbf{c}, \vartheta) = \mu_i^0(\vartheta) + \ln c_i$. Additionally, an *isothermal* system is assumed; hence, $\mu_i^0(\vartheta) = \mu_i^0 \in \mathbb{R}$ is simply a constant;

- the *molar reaction rate* $R_a(\mathbf{c})$ of the a -th reaction is modelled (consistently with the entropy principle) as $R_a(\mathbf{c}) = k_a^f \mathbf{c}^{\alpha^a} - k_a^b \mathbf{c}^{\beta^a}$ with $k_a^f, k_a^b > 0$ satisfying the relation

$$\frac{k_a^f}{k_a^b} = \exp(\langle \mathbf{v}^a, \boldsymbol{\mu}^0 \rangle),$$

for $\boldsymbol{\mu}^0 = (\mu_i^0)_i$.

- Throughout, we assume that all equilibria of the surface chemistry are *detailed-balanced*, i.e.

$$\mathbf{v}^{\Sigma,1}, \dots, \mathbf{v}^{\Sigma,m^\Sigma} \quad \text{are linearly independent.}$$

Then, $\mathbf{e}^k \in \mathbb{R}^N, k = 1, \dots, n^\Sigma := N - m^\Sigma$, characterises linearly independent *conserved quantities* under the surface chemistry, spanning the orthogonal complement of the surface stoichiometric vectors $\{\mathbf{v}^{\Sigma,a} : a = 1, \dots, m^\Sigma\}$.

Moreover, we use the notation $\mathbf{a}^b := (a_1^{b_1}, \dots, a_m^{b_m})$ for any two vectors $\mathbf{a} \in (0, \infty)^k, \mathbf{b} \in \mathbb{R}^k, k \in \mathbb{N}$.

Under these assumptions, and the additional assumption that the sorption processes and surface chemistry take place very fast, i.e. on much smaller time scales than the bulk diffusion and the bulk chemistry, it has been demonstrated in [5] that (GFLM) is a reasonable limit model for the limiting case of infinitely fast surface chemistry and sorption processes (actually, independent of whether one of these two fast thermodynamic mechanism is even ultra-fast), and the condensed form of the limit model (including initial values) reads

$$\partial_t c_i - d_i \Delta c_i = r_i(\mathbf{c}) \quad \text{in } (0, \infty) \times \Omega, \quad i = 1, \dots, N, \tag{1}$$

$$\langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{c} \rangle = 0 \quad \text{on } (0, \infty) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \tag{2}$$

$$k_a^f \prod_{i=1}^N c_i^{\alpha_i^{\Sigma,a}} = k_a^b \prod_{i=1}^N c_i^{\beta_i^{\Sigma,a}} \quad \text{on } (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma = N - n^\Sigma, \quad (3)$$

$$\bar{c}(0, \cdot) = \bar{c}^0, \quad \text{in } (0, \infty) \times \Omega \quad (4)$$

where $\Sigma = \partial\Omega$ denotes the boundary of Ω , acting as an active surface, $\mathbf{D} = \text{diag}(d_1, \dots, d_N)$ is the diagonal matrix of (Fickian) diffusion coefficients, and some initial values $\bar{c}^0 : \bar{\Omega} \rightarrow \mathbb{R}^N$ are given.

4. Local-in-time well-posedness for general bulk and surface chemistry

This section is devoted to the local-in-time well-posedness analysis for generic fast sorption and fast surface chemistry limit models of the form (1)–(4).

Under the imposed modelling assumptions, the system (GFLM) under consideration takes the form:

$$\begin{aligned} \partial_t \bar{c} - \bar{D} \Delta \bar{c} &= \sum_a k_a \left(\exp(\langle \bar{c}^a, \bar{\mu} \rangle) - \exp(\langle \bar{\beta}^a, \bar{\mu} \rangle) \right) \bar{v}^a f && \text{in } (0, \infty) \times \Omega, \\ \langle \bar{e}^k, \bar{D} \partial_n \bar{c} \rangle &= 0 f && \text{on } (0, \infty) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \bar{c}^{\bar{v}^{\Sigma,a}} &= \kappa_a f && \text{on } (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \end{aligned} \quad (5)$$

with the equilibrium constant $\kappa_a = \exp(-\langle \mathbf{v}^{\Sigma,a}, \boldsymbol{\mu}^0 \rangle)$. A possible linearised (around some sufficiently smooth reference vector field $\mathbf{c}^* : (0, \infty) \times \bar{\Omega} \rightarrow (0, \infty)$) version of this nonlinear system is obtained by taking the partial derivatives

$$\frac{\partial}{\partial c_i} \bar{c} |_{\Sigma}^{\bar{v}^{\Sigma,a}} = v_i^\Sigma \frac{1}{c_i |_{\Sigma}} \bar{c} |_{\Sigma}^{\bar{v}^{\Sigma,a}}$$

for $c_i |_{\Sigma} \neq 0$, and reads

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D} \Delta \mathbf{v} &= \mathbf{f} && \text{in } (0, \infty) \times \Omega, \\ \langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{v} \rangle &= g_k && \text{on } (0, \infty) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \sum_{i=1}^N v_i^{\Sigma,a} \frac{v_i}{c_i^*} (\mathbf{c}^*)^{\mathbf{v}^{\Sigma,a}} &= h_a && \text{on } (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \end{aligned}$$

or, for short,

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D} \Delta \mathbf{v} &= \mathbf{f}, && \text{in } (0, \infty) \times \Omega, && \text{(LP)} \\ \langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{v} |_{\Sigma} \rangle &= g_k && \text{on } (0, \infty) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v} |_{\Sigma} \rangle &= h_a && \text{on } (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \end{aligned}$$

where $\mathbf{C}_a^* = (\mathbf{c}^* |_{\Sigma})^{\mathbf{v}^{\Sigma,a}} \text{diag}(c_i^* |_{\Sigma}^{-1})_{i=1}^N : (0, \infty) \times \Sigma \rightarrow \mathbb{R}^{N \times N}$.

Remark 4.1. Since only concentrations $c_i, c_i^\Sigma \geq 0$ have physical significance, only linearisations around states for which all components are (uniformly) strictly positive, i.e. only uniformly strict positive initial values, will be feasible by this approach

towards linearisation. Regularisation effects for reaction–diffusion systems (cf. the strict parabolic maximum principle), however, suggest that this is no severe restriction as (under slight structural assumptions on the chemical reaction network) for any initial values $c_i^0 \geq 0$, but not identically zero, the solution immediately becomes strictly positive, cf. the strict maximum principle for reaction–diffusion equations (see, for example, [18]).

The program of the remainder of this section is the following:

- Show L_p -maximal regularity of the linearised problem, provided sufficient regularity of the reference function c^* . This can be done based on abstract theory in a slightly extended version of the results in [7, 8], or with techniques presented in [14, Chapter 7, Section 10], so that mainly the validity of the Lopatinskiĭ–Shapiro condition and regularity properties have to be checked.
- Use L_p -maximal regularity of the linearised problem and the contraction mapping principle to establish local-in-time existence for the fast sorption and fast surface chemistry limit, provided the initial values are regular enough, have uniformly strictly positive entries and satisfy suitable compatibility conditions.
- Moreover, this procedure will give a “natural” blow-up criterion for global-in-time existence, where by “natural” it is meant that this norm appears in the contraction mapping argument for the local-in-time existence.

4.1. L_p -maximal regularity for the associated linear problem

To show that the linearised problem (LP) possesses the property of L_p -maximal regularity, let us first consider the case of constant coefficients (i.e. a constant reference function $c^* \in (0, \infty)^N$) and a flat boundary (i.e. consider the special case of a boundary $\Sigma = \mathbb{R}^{n-1} \times \{0\}$ for the half-space domain $\Omega = \mathbb{R}^{n-1} \times (0, \infty)$). The corresponding linear initial-boundary value problem to be investigated, on the half-space, then takes the general form of a parabolic reaction–diffusion system with boundary conditions of inhomogeneous type. For technical reasons (unboundedness of the domain Ω), we include a damping constant $\mu \geq 0$. The system then reads as

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D} \Delta \mathbf{v} + \mu \mathbf{v} &= \mathbf{f}, & (t, \mathbf{z}) \in J \times \Omega &= (0, \infty) \times \mathbb{R}^{n-1} \times (0, \infty), \\ \langle \mathbf{e}^k, \mathbf{D} \frac{\partial}{\partial z_n} \mathbf{v} \rangle &= g_k, & (t, \mathbf{z}') \in J \times \Sigma &= (0, \infty) \times \mathbb{R}^{n-1} \times \{0\}, \quad k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma, a}, \mathbf{v} \rangle &= h_a, & (t, \mathbf{z}') \in J \times \Sigma, \quad a &= 1, \dots, m^\Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{v}^0, & \mathbf{z} \in \mathbb{R}^{n-1} \times (0, \infty). \end{aligned} \tag{6}$$

Here, we write $\mathbf{z} = (\mathbf{z}', z_n) \in \mathbb{R}^{n-1} \times \mathbb{R}_+$ for the spatial variables, and the right-hand sides—as the analysis of the linearised problem will reveal—have to satisfy the following regularity conditions:

- (1) $\mathbf{f} \in L_p(J \times \Omega; \mathbb{R}^N)$;
- (2) $\mathbf{g} \in W_p^{(1,2)-(1/2-1/2p)}(J \times \Sigma; \mathbb{R}^{n^\Sigma})$;

- (3) $\mathbf{h} \in W_p^{(1,2) \cdot (1-1/2p)}(J \times \Sigma; \mathbb{R}^{m^\Sigma})$;
- (4) $\mathbf{v}^0 \in W_p^{2-2/p}(\Omega; \mathbb{R}^N)$.

The corresponding maximal regularity result on the half-space reads as follows:

Proposition 4.2 (L_p -maximal regularity on the half-space for constant coefficients). *Assume that $\mathbf{c}^* \in (0, \infty)^N$ is a constant and let $p \in (1, \infty)$. Then, there is $\mu_0 \geq 0$ such that for all $\mu \geq \mu_0$, the half-space problem (6) admits a unique solution $\mathbf{v} \in W_p^{(1,2)}(J \times \Omega; \mathbb{R}^N)$ if and only if $\mathbf{f} \in L_p(J \times \Omega; \mathbb{R}^N)$, $\mathbf{g} \in W_p^{(1,2) \cdot (1/2-1/2p)}(J \times \Sigma; \mathbb{R}^{n^\Sigma})$, $\mathbf{h} \in W_p^{(1,2) \times (1-1/2p)}(J \times \Sigma; \mathbb{R}^{m^\Sigma})$ and $\mathbf{v}^0 \in W_p^{2-2/p}(\Omega; \mathbb{R}^N)$, and, moreover, the following compatibility conditions are satisfied, if the respective time traces exist:*

$$\begin{aligned} \langle \mathbf{e}^k, \mathbf{D} \frac{\partial}{\partial z_n} \mathbf{v}^0 \rangle &= g_k|_{t=0}, & \mathbf{z}' \in \mathbb{R}^{n-1}, k = 1, \dots, n^\Sigma, & \quad (\text{if } p > 3), \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v}^0|_\Sigma \rangle &= h_a|_{t=0}, & \mathbf{z}' \in \mathbb{R}^{n-1}, a = 1, \dots, m^\Sigma, & \quad (\text{if } p > \frac{3}{2}). \end{aligned}$$

In this case, there is $C = C(p, \mu) > 0$, independent of the boundary and initial values, such that

$$\|\mathbf{v}\|_{W_p^{(1,2)}} \leq C(p, \mu) \left(\|\mathbf{f}\|_{L_p} + \|\mathbf{g}\|_{W_p^{(1,2) \cdot (1/2-1/2p)}} + \|\mathbf{h}\|_{W_p^{1-1/2p}} + \|\mathbf{v}^0\|_{W_p^{2-2/p}} \right).$$

Proof. Starting with the system of PDEs (6), taking the partial Laplace–Fourier transform \mathcal{F} for $(\lambda, \xi') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}$, and setting $y = z_n$, leads (formally) to the following parameter-dependent initial value problems

$$\begin{aligned} (\lambda + d_i |\xi'|^2) \hat{v}_i - d_i \frac{\partial^2}{\partial y^2} \hat{v}_i & & (\lambda, \xi', y) \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1} \times (0, \infty), i = 1, \dots, N, \\ + \mu \hat{v}_i(\lambda, \xi', y) &= \hat{f}_i(\lambda, \xi', y), & (\lambda, \xi') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}, k = 1, \dots, n^\Sigma, & \quad (7) \\ \langle \mathbf{e}^k, \mathbf{D} \frac{\partial}{\partial y} \hat{\mathbf{v}}(\lambda, \xi', 0) \rangle &= \hat{g}_k(\lambda, \xi'), & (\lambda, \xi') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}, a = 1, \dots, m^\Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \hat{\mathbf{v}}(\lambda, \xi') \rangle &= \hat{h}_a(\lambda, \xi'), & (\lambda, \xi') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1} \times (0, \infty), \\ \hat{\mathbf{v}}(0, \xi, y) &= \hat{\mathbf{v}}^0(\xi, y), & \end{aligned}$$

where $\hat{v}_i = \mathcal{F} v_i$, $\hat{f}_i = \mathcal{F} f_i$ etc. For fixed $(\lambda, \xi) \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1} \setminus \{(0, \mathbf{0})\}$, the general solution to the ODE in the first line of this system is

$$\begin{aligned} \hat{v}_i(\lambda, \xi', y) &= \exp\left(\left(\left(\frac{\lambda+\mu}{d_i} + |\xi'|^2\right)^{1/2}\right)y\right) \hat{v}_{i,+}(\lambda, \xi') \\ &\quad + \exp\left(\left(-\left(\frac{\lambda+\mu}{d_i} + |\xi'|^2\right)^{1/2}\right)y\right) \hat{v}_{i,-}(\lambda, \xi'). \end{aligned}$$

As we look for a solution in the class $v_i = \mathcal{F}^{-1}(\hat{v}_i) \in L_p((0, T); L_p(\mathbb{R}^{n-1} \times (0, \infty)))$, one necessarily needs to have $\lim_{y \rightarrow \infty} \hat{v}_i(\lambda, \xi', y) = 0$ and hence, (provided the square root $z^{1/2}$ is chosen such that $\Re z^{1/2} > 0$ for all $z \in \overline{\mathbb{C}_0^+}$) $\hat{v}_{i,+}(\lambda, \xi') = 0$ for a.e. $(\lambda, \xi') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}$, and in that case

$$d_i \frac{\partial}{\partial y} \hat{v}_i(\lambda, \xi', 0) = -d_i \left(\left(\frac{\lambda+\mu}{d_i} + |\xi'|^2 \right)^{1/2} \right) \hat{v}_i(\lambda, \xi', 0).$$

To match the solution with the boundary conditions at $\Sigma = \mathbb{R}^{n-1} \times \{0\}$, we thus need to solve the linear system

$$\begin{aligned}
 -\langle \mathbf{e}^k, \mathbf{D}\mathbf{R}\mathbf{v}(\lambda, \boldsymbol{\xi}', 0) \rangle &= \hat{g}_k(\lambda, \boldsymbol{\xi}'), & (\lambda, \boldsymbol{\xi}') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}, \quad k = 1, \dots, n^\Sigma, \\
 \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v}(\lambda, \boldsymbol{\xi}', 0) \rangle &= \hat{h}_a(\lambda, \boldsymbol{\xi}'), & (\lambda, \boldsymbol{\xi}') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}, \quad a = 1, \dots, m^\Sigma,
 \end{aligned}$$

where $\mathbf{R} = \text{diag} \left(\left(\frac{\lambda + \mu}{d_i} + |\boldsymbol{\xi}'|^2 \right)^{1/2} \right)_{i=1}^N$. This system is uniquely solvable for all $(\lambda, \boldsymbol{\xi}') \in \overline{\mathbb{C}_0^+} \times \mathbb{R}^{n-1}$ if and only if the matrix

$$\mathbf{M} = \begin{bmatrix} (\mathbf{e}^1)^\top \\ \vdots \\ (\mathbf{e}^{n^\Sigma})^\top \\ (\mathbf{D}^{-1} \mathbf{R}^{-*} \mathbf{C}_1^* \mathbf{v}^{\Sigma,1})^\top \\ \vdots \\ (\mathbf{D}^{-1} \mathbf{R}^{-*} \mathbf{C}_{m^\Sigma}^* \mathbf{v}^{\Sigma,m^\Sigma})^\top \end{bmatrix} \in \mathbb{C}^{N \times N} \text{ is invertible.}$$

All matrices \mathbf{D} , \mathbf{R} and \mathbf{C}_a^* are diagonal and the matrices

$$\mathbf{C}_a^* = (\mathbf{c}^*|_\Sigma)^{\mathbf{v}^{\Sigma,a}} \tilde{\mathbf{C}}, \quad a = 1, \dots, m$$

coincide with the $N \times N$ diagonal matrix $\tilde{\mathbf{C}} = \text{diag}(c_i^*|_\Sigma)_{i=1, \dots, N}^{-1}$ up to a nonzero factor $(\mathbf{c}^*|_\Sigma)^{\mathbf{v}^{\Sigma,a}}$. The matrix \mathbf{M} is invertible if and only if

$$\begin{bmatrix} (\tilde{\mathbf{D}} \mathbf{v}^{\Sigma,1})^\top \\ \vdots \\ (\tilde{\mathbf{D}} \mathbf{v}^{\Sigma,m^\Sigma})^\top \\ (\mathbf{e}^1)^\top \\ \vdots \\ (\mathbf{e}^{n^\Sigma})^\top \end{bmatrix} \in \mathbb{C}^{N \times N} \text{ is invertible,}$$

where $\tilde{\mathbf{D}} = \mathbf{D}^{-1} \mathbf{R}^{-*} \tilde{\mathbf{C}}$ is an $N \times N$ diagonal matrix with entries $[\tilde{\mathbf{D}}]_{ii} \in \mathbb{C}_0^+$ on the diagonal. Due to Lemma 4.3, this is the case. Using the inverse partial-Fourier-Laplace transformation \mathcal{F}^{-1} , system (6) for $\mathbf{f} = \mathbf{0}$ thus has a unique solution which is given by

$$\begin{aligned}
 \mathbf{v}(t, x', y) &= \mathcal{F}^{-1}(\hat{\mathbf{v}})(t, x', y) \\
 &= \mathcal{F}^{-1} \left(\text{diag} \left(\exp \left(- \left(\frac{\lambda + \mu}{d_i} + |\boldsymbol{\xi}'|^2 \right)^{1/2} y \right) \right) \mathbf{R}^{-1} \mathbf{D}^{-1} \mathbf{M}^{-1} \begin{pmatrix} -\hat{\mathbf{g}} \\ \hat{\mathbf{h}} \end{pmatrix} \right) (t, x', y) \\
 &=: \mathcal{F}^{-1} \left(\hat{\mathbf{T}}_{\lambda, \mu}(\boldsymbol{\xi}', y) \mathbf{R}^{-1} \mathbf{D}^{-1} \mathbf{M}^{-1} \begin{pmatrix} -\hat{\mathbf{g}} \\ \hat{\mathbf{h}} \end{pmatrix} \right) (t, x', y).
 \end{aligned}$$

By Duhamel’s formula, the general solution of (6) is then given by

$$v(t, x', y) = \mathcal{F}^{-1}(\hat{T}_{\lambda, \mu}(\xi', y) \mathbf{R}^{-1} \mathbf{D}^{-1} \mathbf{M}^{-1} \begin{pmatrix} -\hat{g} \\ \hat{h} \end{pmatrix}) + (\hat{T}_{\lambda, \mu} * \hat{f})(\xi', y)(t, x', y),$$

where $*$ denotes convolution with respect to the variable $y > 0$, and v lies in $W_p^{(1,2)}(\mathbb{R}_+ \times \mathbb{R}^n)$, provided $\mu \geq \mu_0$ and $\mu_0 \geq 0$ is chosen sufficiently large. This solves the problem of L_p -maximal regularity for the constant coefficient case on the half-space. \square

For validation of the Lopatinskii–Shapiro condition, we employed the following:

Lemma 4.3. *Let $s, m \in \mathbb{N}$ and $N = s + m$. Let $v^1, \dots, v^m \in \mathbb{R}^N$ and $w^1, \dots, w^s \in \mathbb{R}^N$ be linearly independent, real vectors such that*

$$\langle v^i, w^j \rangle = 0, \quad i = 1, \dots, m, \quad j = 1, \dots, s.$$

Let $\delta_j \in \mathbb{C}$, $j = 1, \dots, N$, be such that $0 \notin \text{conv}\{\delta_j : j = 1, \dots, N\}$ and the matrix $\mathbf{M} \in \mathbb{C}^{N \times N}$ be defined as

$$\vec{\mathbf{M}} = \begin{bmatrix} (\vec{D}\vec{v}^1)^\top \\ \vdots \\ (\vec{D}\vec{v}^m)^\top \\ (\vec{w}^1)^\top \\ \vdots \\ (\vec{w}^s)^\top \end{bmatrix} \quad \text{where } \vec{D} = \text{diag}(\delta_1, \dots, \delta_N) \in \mathbb{C}^{N \times N}.$$

Then, \mathbf{M} is invertible, i.e. $Dv^1, \dots, Dv^m, w^1, \dots, w^s$ form a basis of \mathbb{C}^N .

Proof. As $\mathbf{M} \in \mathbb{C}^{N \times N}$ is a square matrix, it suffices to demonstrate injectivity of \mathbf{M} . Let $u \in N(\mathbf{M})$. Then, in particular,

$$0 = [\mathbf{M}u]_{m+j} = \sum_{i=1}^N w_i^j u_i, \quad \text{i.e. } u \perp w^j, \quad j = 1, \dots, s.$$

Therefore, there are $\gamma_i \in \mathbb{C}$, $i = 1, \dots, m$, such that

$$u = \sum_{i=1}^m \gamma_i v^i.$$

Writing $V = [v^1 \dots v^m] \in \mathbb{R}^{N \times m}$, from $\mathbf{M}u = 0$ it follows $V^\top Du = 0$, thus

$$0 = V^\top Du = V^\top DV\gamma, \quad \text{for } \gamma = (\gamma_1, \dots, \gamma_m)^\top \in \mathbb{C}^m.$$

In particular, since $V^\top = V^*$ (as V has real entries), for the inner product on \mathbb{C}^m one finds

$$0 = \langle \vec{V}^\top D \vec{V} \vec{\gamma}, \vec{\gamma} \rangle_{\mathbb{C}^m} = \langle \vec{D} \vec{V} \vec{\gamma}, \vec{V} \vec{\gamma} \rangle_{\mathbb{C}^m} = \sum_{i=1}^m \delta_i \left| (\vec{V} \vec{\gamma})_i \right|^2.$$

As $|(V\boldsymbol{\gamma})_i|^2 \geq 0$ and $0 \notin \text{conv}\{\delta_i : i = 1, \dots, m\}$, this can only hold true if $\mathbf{u} = V\boldsymbol{\gamma} = \mathbf{0}$, hence \mathbf{M} is injective. \square

The general L_p -maximal regularity theorem (for bounded C^2 -domains Ω) can then be derived via the standard technique, i.e. first a generalisation to the bend-space problem and, thereafter, a localisation procedure. For these techniques to work properly, one needs additional conditions on the (then non-constant) reference function $\mathbf{c}^* : \bar{\Omega} \rightarrow \mathbb{R}^N$. In our case, the bulk diffusion operator $-D\Delta$ does not depend on the spatial position $\mathbf{z} \in \Omega$. Therefore, there is no need to consider perturbations of it, i.e. $\mathcal{A}^{sm} = 0$ in the language of [7,8]. Neither do the conserved quantities \mathbf{e}^k , $k = 1, \dots, n^\Sigma$, but only the matrix $\tilde{\mathbf{C}}(\mathbf{z}) = \text{diag}(\mathbf{c}^*|_\Sigma)^{-1}(\mathbf{z})$ (which is \mathbf{C}_a^* up to an a -dependent factor $(\mathbf{c}^*|_\Sigma)^{\nu^{\Sigma,a}}$) depends on the spatial position $\mathbf{z} \in \bar{\Omega}$. Using the same strategy as in [7], one may write

$$\begin{aligned} \langle \mathbf{C}_a^*(\mathbf{z})\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v}|_\Sigma \rangle &= \langle \mathbf{C}_a^*(\mathbf{z}_0)\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v} \rangle + \langle (\mathbf{C}_a^*(\mathbf{z}) - \mathbf{C}_a^*(\mathbf{z}_0))\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v} \rangle \\ &=: \langle \mathbf{C}_a^*(\mathbf{z}_0)\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v} \rangle + \langle \mathbf{C}_a^{\text{small}}(\mathbf{z})\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v} \rangle, \end{aligned}$$

where $\mathbf{C}_a^{\text{small}}(\mathbf{z})$ corresponds to a *small* perturbation of $\mathbf{C}_a^*(\mathbf{z}_0)$. As in [7], one may then consider the problem

$$\begin{aligned} (\lambda - D\Delta)\mathbf{v}(\lambda, \mathbf{z}) &= f(\lambda, \mathbf{z}), & \lambda \in \overline{\mathbb{C}_0^+}, \mathbf{z} \in \mathbb{R}^{n-1} \times (0, \infty), \\ \langle \mathbf{e}^k, \mathbf{D} \frac{\partial}{\partial \mathbf{y}} \hat{\mathbf{v}}(\lambda, \mathbf{z}', 0) \rangle &= 0, & \lambda \in \overline{\mathbb{C}_0^+}, \mathbf{z}' \in \mathbb{R}^{n-1}, k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}_a^*\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v}(\lambda, \mathbf{z}', 0) \rangle &= -\langle \mathbf{C}_a^{\text{small}}\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v}(\lambda, \mathbf{z}', 0) \rangle, & \lambda \in \overline{\mathbb{C}_0^+}, \mathbf{z}' \in \mathbb{R}^{n-1}. \end{aligned}$$

Letting $A_0 = -D\Delta$ on the domain

$$\begin{aligned} D(A_0) = \left\{ \mathbf{v} \in \mathbf{W}_p^2(\Omega; \mathbb{R}^N) : \left\langle \mathbf{e}^k \mathbf{D} \frac{\partial}{\partial \mathbf{y}} \mathbf{v}|_\Sigma \right\rangle = 0 \right. \\ \left. (k = 1, \dots, n^\Sigma), \langle \mathbf{C}\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v}|_\Sigma \rangle = 0 \quad (a = 1, \dots, m^\Sigma) \right\}, \end{aligned}$$

one then derives a fixed point equation of the form:

$$\mathbf{v} = (\lambda + A_0)^{-1} f - \sum_{j=1}^m S_\lambda^j \langle \mathbf{C}^{\text{small}}\boldsymbol{\nu}^{\Sigma,a}, \mathbf{v}|_\Sigma \rangle.$$

Proceeding as in [8], cf. the upcoming paper [4], one finds that one should demand the following regularity of $\tilde{\mathbf{C}}$, hence of \mathbf{c}^* :

There are $s, r \geq p$ with $\frac{1}{s} + \frac{n-1}{2r} < 1 - \frac{1}{2p}$ such that

$$\begin{aligned} \tilde{\mathbf{C}} \in \mathbf{W}_{s,r}^{(1,2)\cdot(1-1/2p)}(J \times \Sigma; \mathbb{R}^{N \times N}) &:= \mathbf{W}_s^{1-1/2p} \\ & (J; \mathbf{L}_r(\Sigma; \mathbb{R}^{N \times N})) \cap \mathbf{L}_s(J; \mathbf{W}_r^{2-1/p}(\Sigma; \mathbb{R}^{N \times N})), \end{aligned}$$

hence, the reference function \mathbf{c}^* should be *uniformly positive* and

$$\begin{aligned} \mathbf{c}^* &\in W_{s,r}^{(1,2)\cdot(1-1/2p)}(J \times \Sigma; \mathbb{R}^N) \\ &:= W_s^{1-1/2p}(J; L_r(\Sigma; \mathbb{R}^N)) \cap L_s(J; W_r^{2-1/p}(\Sigma; \mathbb{R}^N)). \end{aligned}$$

Details will be provided in [4].

Remark 4.4. Note that for regularity of $\tilde{\mathbf{C}}$, one has to consider the regularity of the functions $(c_k^*)^{-1}$, hence of

$$\frac{\partial}{\partial t} \frac{1}{c_k^*} = -\frac{\partial_t c_k^*}{(c_k^*)^2}, \quad \frac{\partial}{\partial z_i} \frac{1}{c_k^*} = -\frac{\partial_{z_i} c_k^*}{(c_k^*)^2}, \quad \frac{\partial^2}{\partial z_i \partial z_j} \frac{1}{c_k^*} = -\frac{\partial_{z_i} \partial_{z_j} c_k^*}{(c_k^*)^2} - 2\frac{\partial_{z_i} c_k^* \partial_{z_j} c_k^*}{(c_k^*)^3}.$$

Provided $c_k^* \geq \varepsilon > 0$ is (a.e.) uniformly positive, this implies that

$$\|1/c_k^*\|_{W_p^{(1,2)}(J \times \Omega)} \lesssim \frac{1}{\varepsilon} + \frac{1}{\varepsilon^2} \|c_k^*\|_{W_p^{(1,2)}(J \times \Omega)} + \frac{1}{\varepsilon^3} \|\nabla c_k^*\|^2_{L_p(J \times \Omega)},$$

where, provided $W_p^2(\Omega) \hookrightarrow L_{2p}(\Omega)$ (which is true for $p \geq \frac{n}{4}$), $\|\nabla c_k^*\|^2_{L_p(J \times \Omega)} \lesssim \|c_k^*\|^2_{L_p(J; W_p^2(\Omega))}$. Hence, for $p \geq n$, it follows from $c_k^* \in W_p^{(1,2)}(J \times \Omega)$ and $c_k^* \geq \varepsilon > 0$ that $1/c_k^* \in W_p^{(1,2)}(J \times \Omega)$ as well.

Since the reference function should lie in the function class $\mathbf{c}^* \in W_p^{(1,2)\cdot(1-1/2p)}(J \times \Sigma; \mathbb{R}^N)$ and be uniformly positive, one naturally may take $s = r = p$ (other choices are possible as long as the parabolic Sobolev index stays the same, namely $2 - \frac{n+2}{p}$), and then the condition on the values of s and r (here, both equal p) reads

$$\frac{n+1}{2p} < 1 - \frac{1}{2p} \Leftrightarrow p > \frac{n+2}{2}.$$

Note that in this case the embeddings $W_p^{(1,2)}(J \times \Omega) \hookrightarrow C(\bar{J} \times \bar{\Omega})$ and $W_p^{2-2/p}(\Omega) \hookrightarrow C(\bar{\Omega})$ are continuous.

Theorem 4.5. *Let $p > \frac{n+2}{2}$ and $\mathbf{c}^* \in W_p^{(1,2)}(J \times \Omega; (0, \infty)^N)$, where $J = (0, T)$ for some $T > 0$ and $\Omega \subseteq \mathbb{R}^n$ is a bounded C^2 -domain. Then, the linearised problem*

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D} \Delta \mathbf{v} &= \mathbf{f}, & (t, \mathbf{z}) \in (0, \infty) \times \Omega, \\ \langle \mathbf{e}^k, \mathbf{D} \frac{\partial}{\partial \mathbf{n}} \mathbf{v} \rangle &= g_k, & (t, \mathbf{z}) \in (0, \infty) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}^* \mathbf{v}^{\Sigma, a}, \mathbf{v}|_\Sigma \rangle &= h_a, & (t, \mathbf{z}) \in (0, \infty) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{v}^0, & \mathbf{z} \in \Omega \end{aligned}$$

has a unique solution in the function class $\mathbf{v} \in W_p^{(1,2)}(J \times \Omega; \mathbb{R}^N)$ if the data are subject to the following regularity and compatibility conditions:

- (1) $\mathbf{f} \in L_p(J \times \Omega; \mathbb{R}^N) = L_p(J; L_p(\Omega; \mathbb{R}^N))$,

- (2) $g \in W_p^{(1,2) \cdot (1/2-1/2p)}(J \times \Sigma; \mathbb{R}^{n^\Sigma}) = W_p^{1/2-1/2p}(J; L_p(\Sigma; \mathbb{R}^{n^\Sigma})) \cap L_p(J; W_p^{1-1/p}(\Sigma; \mathbb{R}^{n^\Sigma}))$,
- (3) $h \in W_p^{(1,2) \cdot (1-1/2p)}(J \times \Sigma) = W_p^{1-1/2p}(J; L_p(\Sigma; \mathbb{R}^{m^\Sigma})) \cap L_p(J; W_p^{2-1/p}(\Sigma; \mathbb{R}^{m^\Sigma}))$,
- (4) $v^0 \in W_p^{2-2/p}(\Omega; \mathbb{R}^N)$,
- (5) $\langle C_a^* v^{\Sigma, a}, v^0 |_\Sigma \rangle = h_a |_{t=0}$,
- (6) $\langle e^k, D_{\frac{\partial}{\partial n}} v^0 |_\Sigma \rangle = g_k |_{t=0}$ (if $p > 3$).

In this case, the solution depends continuously on the data, i.e. for some $C = C(n, \Omega) > 0$ independent of the data it holds that

$$\|v\|_{W_p^{(1,2)}} \leq C \left(\|f\|_{L_p} + \|g\|_{W_p^{(1,2) \cdot (1/2-1/2p)}} + \|h\|_{W_p^{(1,2) \cdot (1-1/2p)}} + \|v^0\|_{W_p^{2-2/p}(\Omega)} \right).$$

A proof of this result will follow from a subsequent paper on the extension of the abstract results in [7, 8] to the case of combined type boundary conditions, see [4].

More precisely, the following result will be demonstrated in [4].

Theorem 4.6. (*L_p-maximal regularity*) *Let E be a Banach space of class HT, m ∈ N and Ω ⊆ Rⁿ be a domain with compact boundary of class ∂Ω ∈ C^{2m}. For j = 1, . . . , m let m_j ∈ N₀ and linear, continuous projections P_{j,k} ∈ B(E) such that P_{j,k}P_{j,k'} = 0 for k ≠ k' and E = ⊕_{k=0}^{m_j} R(P_{j,k}) for every j = 1, . . . , m_j, be given. Let p ∈ (1, ∞) and suppose that assumptions (E), (LS), (SD), (SB) and (RB) hold true:*

Let linear differential operators A(t, x, D) and B_j(t, x, D) and their principle parts be defined via their symbols

$$A(t, z, \vec{\xi}) = \sum_{|\vec{\alpha}| \leq 2m} \alpha_{\vec{\alpha}}(t, z) \vec{\xi}^{\vec{\alpha}}, \quad B_j(t, z, \vec{\xi}) = \sum_{k=0}^{m_j} \sum_{|\vec{\beta}| \leq k} \beta_{j,k,\vec{\beta}}(t, z) \vec{\xi}^{\vec{\beta}} P_{j,k}.$$

(E) *Ellipticity of the interior symbol: For all t ∈ J, z ∈ Ω̄ and ξ̄ ∈ Sⁿ⁻¹ it holds that*

$$\sigma(A(t, z, \xi)) \subseteq \mathbb{C}_0^+,$$

i.e. A(t, z, D) is normally elliptic. If Ω is unbounded, the same condition is imposed at z = ∞.

(LS) *Lopatinskiĭ–Shapiro condition: For all t ∈ J, z ∈ ∂Ω and all ξ ∈ Rⁿ with ξ · n(z) = 0, and all λ ∈ C₀⁺ such that (λ, ξ) ≠ (0, 0), the initial value problem*

$$\begin{aligned} \lambda v(y) + A_{\#}(t, z, \xi + i n(z) \frac{\partial}{\partial y}) v(y) &= 0, & y > 0, \\ B_{j,\#}(t, z, \xi + i n(z) \frac{\partial}{\partial y}) v(0) &= h_j, & j = 1, \dots, m, \end{aligned}$$

has a unique solution in the class v ∈ C₀(R₊; E).

(SD) There are $r_l, s_l \geq p$ with $\frac{1}{s_l} + \frac{n}{2mr_l} < 1 - \frac{l}{2m}$ such that

$$\begin{aligned} a_\alpha &\in L_{s_l}(J; [\mathbf{L}_{r_l} + \mathbf{L}_\infty](\Omega; \mathcal{B}(E))), & |\alpha| &= l < 2m, \\ a_\alpha &\in C_l(J \times \overline{\Omega}; \mathcal{B}(E)), & |\alpha| &= 2m. \end{aligned}$$

(SB) There are $s_{j,k,l}, r_{j,k,l} \geq p$ with $\frac{1}{s_{j,k,l}} + \frac{n-1}{2mr_{j,k,l}} < \kappa_{j,k} + \frac{l-k}{2m}$ such that

$$b_{j,k,\beta} \in \mathbf{W}_{s_{j,k,l}, r_{j,k,l}}^{(1,2m) \cdot \kappa_{j,k}}(J \times \partial\Omega; \mathcal{B}(E)), \quad |\beta| = l \leq k \leq m_j.$$

(RB) For every $j = 1, \dots, m$ and $k = 0, 1, \dots, m_j$ it holds that

$$b_{j,k,\beta}(\mathbf{R}(\mathcal{P}_{jk})) \subseteq \mathbf{R}(\mathcal{P}_{jk}), \quad |\beta| = k.$$

Then, the problem

$$\begin{aligned} \partial_t u + \mathcal{A}(t, z, D)u &= f(t, z), & t \in J, z \in \Omega, \\ \mathcal{B}_j(t, z, D)u &= g_j(t, z), & t \in J, z \in \partial\Omega, j = 1, \dots, m, \\ u(0, z) &= u_0(z), & z \in \Omega \end{aligned} \tag{8}$$

has a unique solution in the class

$$u \in \mathbf{W}_p^{(1,2m)}(J \times \Omega; E)$$

if and only if the data f, g and u_0 are subject to conditions **(D)** as follows:

(D) Assumptions on the data:

- (i) $f \in L_p(J \times \Omega; E)$,
- (ii) $g_{j,k} \in \mathbf{W}_p^{(1,2m) \cdot \kappa_{j,k}}(J \times \partial\Omega; E)$, where $\kappa_{j,k} = \frac{2m-k-1/p}{2m}$, and we then set $g_j = \sum_{k=0}^{m_j} g_{j,k}$.
- (iii) $u_0 \in \mathbf{W}_p^{2m(1-1/p)}(\Omega; E)$,
- (iv) if $\kappa_{j,k} > 1/p$, then $\mathcal{B}_j(0, z)\mathcal{P}_{j,k}u_0(z) = g_{j,k}(0, z)$ for $z \in \partial\Omega$.

In the concrete situation of this manuscript, we may choose $m = 1$ and $E = \mathbb{R}^N$, $a_\alpha(t, z) = \mathbf{D}$ for $\alpha = 2e_i, i = 1, \dots, N$, and $a_\alpha(t, z) = 0$ otherwise. Moreover $b_{j,1,e_k}(t, z)\mathbf{v} = \langle e^j, \mathbf{v} \cdot \mathbf{D}\mathbf{v} \rangle e_k$ for $k = 1, \dots, n^\Sigma$, and $b_{1,0,0}(t, z)\mathbf{v} = b_{1,1,0}\mathbf{v} = \sum_a \langle \mathbf{C}_a^*(t, z)\mathbf{v}^{\Sigma,a}, \mathbf{v} \rangle e_{n^\Sigma+a}$, $a = 1, \dots, m^\Sigma$. Furthermore, $\mathcal{P}_{1,1}$ is the (orthogonal) projection in \mathbb{R}^N onto $\text{span}\{\mathbf{D}^{-1}e^k : k = 1, \dots, n^\Sigma\}$ and $\mathcal{P}_{1,0}$ is the (orthogonal) projection in \mathbb{R}^N onto $\{\mathbf{D}^{-1}e^k : k = 1, \dots, n^\Sigma\}^\perp$. Thus,

$$\begin{aligned} [\mathcal{B}_1(t, x, D)u]_k &= \langle e^k, \mathbf{v} \cdot \mathbf{D}\nabla(\mathcal{P}_{1,1}u) \rangle + 0 \cdot \mathcal{P}_{1,0}u \\ &= \langle e^k, \mathbf{D}\partial_{\mathbf{v}}u \rangle, \quad k = 1, \dots, n^\Sigma, \\ [\mathcal{B}_1(t, x, D)u]_{n^\Sigma+a} &= \langle \mathbf{C}_a^*(t, z)\mathbf{v}^{\Sigma,a}, u \rangle \mathcal{P}_{1,1} + \langle \mathbf{C}_a^*(t, z)\mathbf{v}^{\Sigma,a}, u \rangle \mathcal{P}_{1,0} \\ &= \langle \mathbf{C}_a^*(t, z)\mathbf{v}^{\Sigma,a}, u \rangle, \quad a = 1, \dots, m^\Sigma = N - n^\Sigma. \end{aligned}$$

As typical for many semi-linear systems, L_p -maximal regularity, and (in this case) L_p - L_q -estimates can be employed to find a (unique) strong solution of the quasi-linear problem. This will be the aim of the next subsection.

4.2. Local-in-time existence of strong solutions, blow-up criteria and a priori bounds

Having maximal regularity for the linearised problem at hand, we may now come back to the semilinear problem. L_p -maximal regularity will play the typically crucial role in the construction of strong solutions via the contraction mapping principle. Thereby, rather as a by-product, a condition for continuation of the solution to a maximal solution will be established, where in general the solution may be global in time (which might be expected for a large subclass of the systems considered here), or one may observe a blow-up in finite time. Whereas the boundedness of the $W_p^{2-2/p}$ -norm cannot be guaranteed in general, or more precisely, it is unclear whether boundedness holds true without any restriction on the bulk and surface chemistry, for slightly weaker norms a priori bounds are possible, indeed. The latter will be considered in the second part of this subsection.

4.2.1. Local-in-time existence and maximal continuation of solutions

Recall the form of the fast sorption and fast surface chemistry limit (5), and additionally consider given initial values $\mathbf{c}^0 : \bar{\Omega} \rightarrow \mathbb{R}^N$ which should be regular enough (in a sense to be made precise later on):

$$\begin{aligned} \partial_t \mathbf{c} - \mathbf{D} \Delta \mathbf{c} &= \sum_a \left(k_a^f \mathbf{c}^{\alpha^a} - k_a^b \mathbf{c}^{\beta^a} \right) \mathbf{v}^a, & (t, z) \in (0, \infty) \times \Omega, & (5') \\ \langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{c} \rangle &= 0, & (t, z) \in (0, \infty) \times \Sigma, k = 1, \dots, n^\Sigma, \\ \mathbf{c}^{\nu^{\Sigma, a}} &= \exp(-\langle \mathbf{v}^{\Sigma, a}, \boldsymbol{\mu}^0(\vartheta) \rangle), & (t, z) \in (0, \infty) \times \Sigma, a = 1, \dots, m^\Sigma, \\ \mathbf{c}|_{t=0} &= \mathbf{c}^0, & z \in \Omega. \end{aligned}$$

Moreover, let $T_0 > 0$ be any fixed, finite time horizon and $\mathbf{c}^* : (0, T_0) \times \Omega \rightarrow \mathbb{R}^N$ be a (sufficiently regular) auxiliary function which admits a time trace and $\mathbf{c}^*|_{t=0} = \mathbf{c}^0$. Introducing $\mathbf{v}(t, z) := \mathbf{c}(t, z) - \mathbf{c}^*(t, z)$ leads to the reaction–diffusion–sorption system for \mathbf{v} as follows:

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D} \Delta \mathbf{v} &= \sum_a \left(k_a^f (\mathbf{v} + \mathbf{c}^*)^{\alpha^a} - k_a^b (\mathbf{v} + \mathbf{c}^*)^{\beta^a} \right) \mathbf{v}^a \\ &\quad - [\partial_t - \mathbf{D} \Delta] \mathbf{c}^* && \text{in } (0, T_0) \times \Omega, \\ \langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{v} \rangle &= -\langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{c}^* \rangle && \text{on } (0, T_0) \times \Sigma, k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma, a}, \mathbf{v} \rangle &= \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma, a}, \mathbf{v} \rangle - (\mathbf{c}^* + \mathbf{v})^{\nu^{\Sigma, a}} + \exp(-\langle \mathbf{v}^{\Sigma, a}, \boldsymbol{\mu}^0(\vartheta) \rangle) && \text{on } (0, T_0) \times \Sigma, a = 1, \dots, m^\Sigma, \\ \mathbf{v}|_{t=0} &= \mathbf{0} && \text{in } \Omega, \end{aligned}$$

where $\mathbf{C}_a^* = (\mathbf{c}^*)^{-\nu^{\Sigma, a}} \text{diag}(\mathbf{c}^*)^{-1} : (0, T_0) \times \Sigma \rightarrow \mathbb{R}^{N \times N}$. Next, assume that $p > \frac{n+2}{2}$, and for $\tau > 0$ consider the nonlinear solution operator

$$\Phi_\tau : D_0 \subseteq W_p^{(1,2)} \left((0, \tau) \times \Omega; \mathbb{R}^N \right) \rightarrow W_p^{(1,2)} \left((0, \tau) \times \Omega; \mathbb{R}^N \right)$$

given by $\mathbf{v} \mapsto \mathbf{w}$, where

$$D_0 = \left\{ \mathbf{v} \in W_p^{(1,2)}((0, \tau) \times \Omega; \mathbb{R}^N) : \mathbf{v}|_{t=0} \equiv \mathbf{0} \right\}$$

and w is the unique strong solution to the linear problem

$$\begin{aligned} \partial_t w - D\Delta w &= \sum_a \left(k_a^f (v + c^*)^{\alpha^a} - k_a^b (v + c^*)^{\beta^a} \right) v^a \\ &\quad - (\partial_t - D\Delta)c^* \quad \text{in } (0, \tau) \times \Omega, \\ \langle e^k, D\partial_n w \rangle &= -\langle e^k, D\partial_n c^* \rangle \quad \text{on } (0, \tau) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \langle C_a^* v^{\Sigma, a}, w \rangle &= \langle C_a^* v^{\Sigma, a}, v \rangle - (c^* + v)^{v^{\Sigma, a}} \\ &\quad + \exp(-\langle v^{\Sigma, a}, \mu^0(\vartheta) \rangle) \quad \text{on } (0, \tau) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \\ w|_{t=0} &= \mathbf{0} \quad \text{in } \Omega. \end{aligned}$$

This problem can now be handled in the way typical for semi-linear parabolic problems, employing the maximal regularity of the linearised problem and the regularity of the nonlinear maps on the right-hand side, which allows for a fixed point argument via the contraction mapping principle. To establish the regularity properties which are needed, one first needs the following auxiliary result on embedding properties of $W_p^{(1,2)}(J \times \Omega)$ for bounded intervals J and bounded C^2 -domains Ω .

Lemma 4.7. *Let $p \in (\frac{n+2}{2}, \infty)$ and $\Omega \subseteq \mathbb{R}^n$ be a bounded C^2 -domain. Fix $T_0 > 0$. For $T \in (0, T_0]$ and*

$$D_0(T) = \mathring{W}_p^{(1,2)}((0, T] \times \overline{\Omega}) := \left\{ u \in W_p^{(1,2)}((0, T) \times \Omega) : u(0) = 0 \right\},$$

the embedding constants for the continuous embeddings

$$D_0(T) \hookrightarrow C(\overline{J} \times \overline{\Omega})$$

can be chosen independently of $T \in (0, T_0)$, e.g. $C_p = 2^{1/p} C_p(T_0)$ where $C_p(T_0)$ is an embedding constant for $T = T_0$.

Proof. Since for $u \in D_0(T)$ one has $u(0) = 0$, it follows that

$$\tilde{u}(t, \cdot) := \begin{cases} u(t, \cdot), & t \in [0, T], \\ u(T - t, \cdot), & t \in (T, 2T], \\ 0, & t > 2T \end{cases}$$

defines a function $\tilde{u} \in W_p^{(1,2)}(\mathbb{R}_+ \times \Omega)$ and for its restriction to $[0, T_0] \times \Omega$ it holds that

$$\begin{aligned} \|\tilde{u}\|_{W_p^{(1,2)}((0, T_0) \times \Omega)} &\leq 2^{1/p} \|u\|_{W_p^{(1,2)}((0, T) \times \Omega)}, \\ \|\tilde{u}\|_\infty &= \|u\|_\infty. \end{aligned}$$

From here the assertion follows easily. □

Theorem 4.8 (Local-in-time existence of strong solutions). *Let $p > \frac{n+2}{2}$ and assume that $\Omega \subseteq \mathbb{R}^n$ is a bounded domain of class $\partial\Omega \in C^2$. Then, the fast sorption and fast surface chemistry limit problem (5') admits a unique local-in-time strong solution, if*

$$\mathbf{c}^0 \in I_p^+(\Omega) := \{\mathbf{c}^0 \in W_p^{2-2/p}(\Omega; (0, \infty)^N) : \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^0|_\Sigma \rangle = 0, \mathbf{c}^0|_\Sigma^{\nu^{\Sigma,a}} = \exp(-\nu^{\Sigma,a} \cdot \boldsymbol{\mu}^0(\vartheta))\}.$$

More precisely, for every reference initial values $\mathbf{c}^{\text{ref}} \in I_p^+(\Omega)$, there are $T > 0$, $\varepsilon > 0$ and $C > 0$ such that the following statements hold true:

- (1) For all $\mathbf{c}^0 \in I_p^+(\Omega)$ with $\|\mathbf{c}^0 - \mathbf{c}^{\text{ref}}\|_{I_p(\Omega)} < \varepsilon$, there is a unique strong solution $\mathbf{c} \in W_p^{(1,2)}(J \times \Omega; (0, \infty)^N)$ of (5') for $J = [0, T]$.
- (2) For any two initial values $\mathbf{c}^0, \tilde{\mathbf{c}}^0 \in I_p^+(\Omega)$ with $\|\mathbf{c}^0 - \mathbf{c}^{\text{ref}}\|_{W_p^{2-2/p}}, \|\tilde{\mathbf{c}}^0 - \mathbf{c}^{\text{ref}}\|_{W_p^{2-2/p}} < \varepsilon$ and corresponding strong solutions $\mathbf{c}, \tilde{\mathbf{c}} \in W_p^{(1,2)}(J \times \Omega; \mathbb{R}^N)$ one has

$$\|\mathbf{c} - \tilde{\mathbf{c}}\|_{W_p^{(1,2)}(J \times \Omega)} \leq C \|\mathbf{c}^0 - \tilde{\mathbf{c}}^0\|_{W_p^{2-2/p}(\Omega)}.$$

- (3) Any strong solution $\mathbf{c} \in W_p^{(1,2)}(J \times \Omega)$ can be extended in a unique way to a maximal (Hölder) strong solution $\mathbf{c} : [0, T_{\max}) \times \Omega \rightarrow (0, \infty)^N$ (with $T_{\max} \in (0, \infty]$), where $\mathbf{c} \in W_p^{(1,2)}((0, T) \times \Omega; (0, \infty)^N)$ for every $T \in (0, T_{\max})$.

Proof. Let $\eta > 0$ and initial values

$$\tilde{\mathbf{c}}^0 \in I_p^\eta(\Omega) := \{\tilde{\mathbf{c}}^0 : c_i^0 \geq \eta \quad (i = 1, \dots, N) \text{ on } \overline{\Omega}\}$$

be given. Let $\rho_0, T_0 > 0$ be such that

$$\|\tilde{\mathbf{v}}\|_\infty \leq \frac{\eta}{4} \quad \text{for all } \tilde{\mathbf{v}} \in D_{\rho,T} := \{\tilde{\mathbf{v}} \in W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N) : \tilde{\mathbf{v}}(0, \cdot) = 0, \|\tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)} \leq \rho\},$$

where $\rho \in (0, \rho_0]$, $T \in (0, T_0]$. (Such a choice is possible, e.g. by Lemma 4.7.) Moreover, let \mathcal{E} be a linear, continuous extension operator from $W_p^{2-2/p}(\Omega)$ to $W_p^{(1,2)}((0, T_0) \times \Omega)$ and from $C(\overline{\Omega})$ to $C([0, T_0] \times \overline{\Omega})$. Moreover, w.l.o.g. assume that $\mathcal{E}\mathbf{v} \geq \frac{\eta}{2}$ on $(0, T_0) \times \Omega$ whenever $\mathbf{v} \geq \eta$ on Ω , and let $\rho_0 \leq \frac{\eta}{3C(T_0)}$ where $C(T_0) > 0$ is a common embedding constant for the continuous embeddings $\dot{W}_p^{(1,2)}((0, T) \times \overline{\Omega}) \hookrightarrow C([0, T] \times \overline{\Omega})$ from Lemma 4.7. Then, $\mathcal{E}\mathbf{c}^0 + \mathbf{v} \geq \frac{\eta}{6}$ for all $\rho \in (0, \rho_0]$, $T \in (0, T_0]$ and $\mathbf{v} \in D_{\rho,T}$ on $(0, T) \times \Omega$.

We are looking for a solution $\mathbf{c} \in W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N)$ of the reaction–diffusion system with linear, combined type boundary conditions

$$\begin{aligned} \partial_t \mathbf{c} - \mathbf{D}\Delta \mathbf{c} &= \mathbf{r}(\mathbf{c}) && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c} \rangle &= 0 && \text{on } (0, T) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \mathbf{c}^{\nu^{\Sigma,a}} &= \kappa_a (> 0) && \text{on } (0, T) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \end{aligned}$$

$$\mathbf{c}(0, \cdot) = \mathbf{c}^0 \quad \text{in } \Omega.$$

We set $\mathbf{c}^* := \mathcal{E}\mathbf{c}^0 \in W_p^{(1,2)}((0, T_0) \times \Omega; \mathbb{R}^N)$ and $\mathbf{v} := \mathbf{c} - \mathbf{c}^*$. Then, in order for \mathbf{c} to be the solution to the reaction–diffusion–sorption system considered here, \mathbf{v} has to be the solution to the following initial-boundary value problem:

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D}\Delta \mathbf{v} &= \mathbf{r}(\mathbf{c}^* + \mathbf{v}) - (\partial_t - \mathbf{D}\Delta)\mathbf{c}^* && \text{in } (0, T) \times \Omega, && (*) \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{v} \rangle &= \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^* \rangle && \text{on } (0, T) \times \Sigma, k = 1, \dots, n^\Sigma, \\ (\mathbf{c}^* + \mathbf{v})^{\nu^{\Sigma,a}} &= \kappa_a && \text{on } (0, T) \times \Sigma, a = 1, \dots, m^\Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{0} && \text{in } \Omega. \end{aligned}$$

To derive a semilinear formulation of this problem, we rewrite the nonlinear boundary conditions on \mathbf{v} as follows. By Taylor's series, we may write

$$(\mathbf{c}^* + \mathbf{v})^{\nu^{\Sigma,a}} = (\mathbf{c}^*)^{\nu^{\Sigma,a}} + \sum_{i=1}^N v_i^{\Sigma,a} v_i \frac{(\mathbf{c}^*)^{\nu^{\Sigma,a}}}{c_i^*} + \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*)$$

for a function \mathcal{Q}_a which is continuously differentiable of arbitrary order, at least on

$$\left\{ (\mathbf{v}, \mathbf{c}^*) \in \mathbb{R}^N \times (0, \infty)^N : v_i + c_i^* > 0 \right\}.$$

Hence, we may express the nonlinear boundary condition $(\mathbf{c}^* + \mathbf{v})^{\nu^{\Sigma,a}} = \kappa_a$ in the equivalent semilinear form

$$\langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v} \rangle = \sum_{i=1}^N v_i^{\Sigma,a} v_i \frac{(\mathbf{c}^*)^{\nu^{\Sigma,a}}}{c_i^*} = \kappa_a - (\mathbf{c}^*)^{\nu^{\Sigma,a}} - \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*).$$

Then, $\mathbf{v} \in D_{\rho,T}$ is a solution $\mathbf{v} \in W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N)$ of (*) if and only if

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D}\Delta \mathbf{v} &= \mathbf{r}(\mathbf{c}^* + \mathbf{v}) - (\partial_t - \mathbf{D}\Delta)\mathbf{c}^* && \text{in } (0, T) \times \Omega, && (**) \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{v} \rangle &= \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^* \rangle && \text{on } (0, T) \times \Sigma, k = 1, \dots, n^\Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v} \rangle &= \kappa_a - (\mathbf{c}^*)^{\nu^{\Sigma,a}} - \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) && \text{on } (0, T) \times \Sigma, a = 1, \dots, m^\Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{0} && \text{in } \Omega. \end{aligned}$$

Therefore, $\mathbf{v} \in D_{\rho,T}$ is a solution to (*), if and only if $\mathbf{v} \in D_{\rho,T}$ is a fixed point of the (well defined, due to the choice of ρ_0, T_0) map $\Phi : D_{\rho,T} \rightarrow W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N)$ defined as follows: For $\mathbf{v} \in D_{\rho,T}$ let $\Phi(\mathbf{v}) := \mathbf{w}$ be the unique solution to the inhomogeneous, parabolic initial-boundary value-problem

$$\begin{aligned} \partial_t \mathbf{w} - \mathbf{D}\Delta \mathbf{w} &= \mathbf{r}(\mathbf{c}^* + \mathbf{v}) - (\partial_t - \mathbf{D}\Delta)\mathbf{c}^* =: \mathbf{f}(\mathbf{c}^*, \mathbf{v}) && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{w} \rangle &= \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^* \rangle =: \mathbf{g}_k(\mathbf{c}^*) && \text{on } (0, T) \times \Sigma, k = 1, \dots, n^\Sigma, \\ \mathbf{C}_a^* \mathbf{v}^{\Sigma,a} \mathbf{w} &= \kappa_a - (\mathbf{c}^*)^{\nu^{\Sigma,a}} - \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) =: \mathbf{h}_a(\mathbf{c}^*, \mathbf{v}) && \text{on } (0, T) \times \Sigma, a = 1, \dots, m^\Sigma, \end{aligned}$$

$$\mathbf{w}(0, \cdot) = \mathbf{0} \quad \text{in } \Omega.$$

By L_p -maximal regularity of the linearised problem, the solution $\mathbf{w} \in W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N)$ exists and is uniquely determined, for every $\mathbf{v} \in D_{\rho, T}$. That is, Φ is well defined. Since the initial values $\mathbf{w}(0, \cdot) = \mathbf{0}$ are zero for all the functions constructed in this way, the constant $C_T = C_{T_0} > 0$ in the maximal regularity estimate

$$\begin{aligned} \|\Phi(\mathbf{v})\|_{W_p^{(1,2)}((0, T) \times \Omega)} &\leq C_{T_0} (\|\mathbf{f}(\mathbf{c}^*, \mathbf{v})\|_{L^p((0, T) \times \Omega)} \\ &\quad + \|\mathbf{g}(\mathbf{c}^*)\|_{W_p^{(1,2) \cdot (1/2-1/2p)}((0, T) \times \Sigma)} + \|\mathbf{h}(\mathbf{c}^*, \mathbf{v})\|_{W_p^{(1,2) \cdot (1-1/2p)}((0, T) \times \Sigma)}) \end{aligned}$$

for $\mathbf{v} \in D_{\rho, T}$ can be chosen independently of $T \in (0, T_0]$. This can be seen, for example, by using the following mirroring type argument: Set

$$\begin{aligned} \tilde{\mathbf{f}}(t, \cdot) &= \begin{cases} \mathbf{f}(t, \cdot), & t \in [0, T], \\ \mathbf{0}, & t > T, \end{cases}, \quad \tilde{\mathbf{g}}(t, \cdot) = \begin{cases} \mathbf{g}(t, \cdot), & t \in [0, T], \\ \mathbf{g}(2T - t, \cdot), & t \in (T, 2T), \\ \mathbf{0}, & t > 2T, \end{cases} \\ \tilde{\mathbf{h}}(t, \cdot) &= \begin{cases} \mathbf{h}(t, \cdot), & t \in [0, T], \\ \mathbf{h}(2T - t, \cdot), & t \in (T, 2T), \\ \mathbf{0}, & t > 2T, \end{cases} \end{aligned}$$

and consider the problem with time horizon T_0 :

$$\begin{aligned} \partial_t \mathbf{w} - \mathbf{D} \Delta \mathbf{w} &= \tilde{\mathbf{f}} && \text{in } (0, T_0) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{w} \rangle &= \tilde{g}_k && \text{on } (0, T_0) \times \Sigma, \quad k = 1, \dots, n^\Sigma, \\ \mathbf{C}_a^* \mathbf{v}^{\Sigma, a} \mathbf{w} &= \tilde{h}_a && \text{on } (0, T_0) \times \Sigma, \quad a = 1, \dots, m^\Sigma, \\ \mathbf{w}(0, \cdot) &= \mathbf{0} && \text{in } \Omega. \end{aligned}$$

Then, there is a constant $C = C(T_0)$ (from L_p -maximal regularity) such that

$$\begin{aligned} \|\mathbf{w}\|_{W_p^{(1,2)}((0, T_0) \times \Omega)} &\leq C (\|\tilde{\mathbf{f}}\|_{L^p((0, T_0) \times \Omega)} + \|\tilde{\mathbf{g}}\|_{W_p^{(1,2) \cdot (1/2-1/2p)}((0, T_0) \times \Sigma)} \\ &\quad + \|\tilde{\mathbf{h}}\|_{W_p^{(1,2) \cdot (1-1/2p)}((0, T_0) \times \Sigma)}). \end{aligned}$$

Then, by construction (and uniqueness of solutions), $\mathbf{w}|_{[0, T] \times \Omega}$ is the solution to the problem with time horizon $T \in (0, T_0]$ for the given data $(\mathbf{f}, \mathbf{g}, \mathbf{h})$ and

$$\begin{aligned} \|\mathbf{w}|_{[0, T] \times \Omega}\|_{W_p^{(1,2)}((0, T) \times \Omega)} &\leq \|\mathbf{w}\|_{W_p^{(1,2)}((0, T_0) \times \Omega)} \\ &\leq C \left(\|\tilde{\mathbf{f}}\|_{L^p((0, T_0) \times \Omega)} + \|\tilde{\mathbf{g}}\|_{W_p^{(1,2) \cdot (1/2-1/2p)}((0, T_0) \times \Sigma)} + \|\tilde{\mathbf{h}}\|_{W_p^{(1,2) \cdot (1-1/2p)}((0, T_0) \times \Sigma)} \right) \\ &\leq 2^{1/p} C \left(\|\mathbf{f}\|_{L^p((0, T_0) \times \Omega)} + \|\mathbf{g}\|_{W_p^{(1,2) \cdot (1/2-1/2p)}((0, T_0) \times \Sigma)} + \|\mathbf{h}\|_{W_p^{(1,2) \cdot (1-1/2p)}((0, T_0) \times \Sigma)} \right). \end{aligned}$$

We will demonstrate that $\rho \in (0, \rho_0]$ and $T \in (0, T_0]$ can be chosen such that Φ is a contractive self-mapping on $D_{\rho, T}$, and hence attains a unique fixed point by the

contraction mapping principle. To this end, we show that for suitably small $\rho \in (0, \rho_0]$ and $T \in (0, T_0]$, Φ is a strictly contractive mapping from $D_{\rho, T}$ into $D_{\rho, T}$.

First, note that since $\|\mathbf{v}\|_\infty \leq \frac{\eta}{3}$ for every $\mathbf{v} \in D_{\rho, T}$ with $\rho \in (0, \rho_0]$, $T \in (0, T_0]$, we may denote by $\|\mathbf{r}\|$ and $\|\mathcal{Q}_a\|$ the respective norms as functions on $[\frac{\eta}{6}, \|\mathbf{c}^*\|_\infty + \frac{\eta}{4}]^N$. Secondly, we will frequently use that $\mathbf{v}(0, \cdot) = \tilde{\mathbf{v}}(0, \cdot) \equiv \mathbf{0}$, $\mathbf{g}(\mathbf{c}^*)|_{t=0} = \mathbf{g}(\mathbf{c}^0) \equiv \mathbf{0}$ (as \mathbf{c}^0 satisfies the compatibility conditions) and $\mathbf{h}(\mathbf{c}^*, \mathbf{v}) = \mathbf{h}(\mathbf{c}^*, \tilde{\mathbf{v}}) \equiv \mathbf{0}$. Therefore, for every $\mathbf{v}, \tilde{\mathbf{v}} \in D_{\rho, T}$ and $\rho \in (0, \rho_0]$, $T \in (0, T_0]$, and after fixing some auxiliary value $\tilde{p} \in (n+2/2, p)$, hence $\dot{W}_{\tilde{p}}^{(1,2)}((0, T] \times \bar{\Omega}) \hookrightarrow C([0, T] \times \bar{\Omega})$ with an embedding constant $C(T_0)$ that can be used uniformly for all $T \in (0, T_0]$, we obtain estimates

$$\begin{aligned} \|\mathbf{r}(\mathbf{c}^* + \mathbf{v})\|_{L_p((0,T) \times \Omega)} &\leq (T |\Omega|)^{1/p} \|\mathbf{r}\|_\infty, \\ \|\mathbf{r}(\mathbf{c}^* + \mathbf{v}) - \mathbf{r}(\mathbf{c}^* + \tilde{\mathbf{v}})\|_{L_p((0,T) \times \Omega)} &\leq \|\mathbf{r}'\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\ &= \|\mathbf{r}'\|_\infty \left(\int_0^T \left\| \int_0^t \partial_t \mathbf{v}(s, \cdot) - \partial_t \tilde{\mathbf{v}}(s, \cdot) \, ds \right\|_{L_p(\Omega)}^p dt \right)^{1/p} \\ &\leq \|\mathbf{r}'\|_\infty T^{1/p} \|\partial_t \mathbf{v} - \partial_t \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\ &\leq \|\mathbf{r}'\|_\infty T^{1/p} \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)}, \\ \|\mathbf{g}_k(\mathbf{c}^*)\|_{W_p^{(1,2),(1/2-1/2p)}((0,T) \times \Sigma)} &\leq C \|\partial_n \mathbf{c}^*\|_{W_p^{(1,2),(1/2-1/2p)}((0,T) \times \Sigma)}, \\ \|h_a(\mathbf{c}^*, \mathbf{v})\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)} &\leq \|(\mathbf{c}^*)^{\mathbf{v}^{\Sigma, a}} - \kappa_a\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)} \\ &\quad + \|\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*)\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)}, \\ \|h_a(\mathbf{c}^*, \mathbf{v}) - h_a(\mathbf{c}^*, \tilde{\mathbf{v}})\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)} \\ &= \|\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) - \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*)\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)}. \end{aligned}$$

Here, the critical terms in the estimates for the norms of h_a can be estimated as follows:

$$\begin{aligned} \|\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) - \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*)\|_{W_p^{(1,2),(1-1/2p)}((0,T) \times \Sigma)} \\ \leq C(T_0) \|\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) - \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*)\|_{W_p^{(1,2)}((0,T) \times \Omega)} \quad \text{as } \mathbf{v}|_{t=0} = \tilde{\mathbf{v}}|_{t=0} = \mathbf{0}, \quad \text{with} \\ \|\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) - \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \leq \|\partial_v \mathcal{Q}_a\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\ \leq \|\partial_v \mathcal{Q}_a\|_\infty (T |\Omega|)^{1/p} \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)}; \end{aligned}$$

and for the time derivative

$$\begin{aligned} \|\partial_t(\mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) - \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*))\|_{L_p((0,T) \times \Omega)} \\ \leq \|\partial_v \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) \cdot \partial_t \mathbf{v} - \partial_v \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*) \cdot \partial_t \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\ + \|\partial_{\mathbf{c}^*} \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) \cdot \partial_t \mathbf{c}^* - \partial_{\mathbf{c}^*} \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*) \cdot \partial_t \mathbf{c}^*\|_{L_p((0,T) \times \Omega)} \\ \leq \|\partial_v \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) \cdot (\partial_t \mathbf{v} - \partial_t \tilde{\mathbf{v}})\|_{L_p((0,T) \times \Omega)} + \|(\partial_v \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) \\ - \partial_v \mathcal{Q}_a(\tilde{\mathbf{v}}, \mathbf{c}^*)) \cdot \partial_t \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \end{aligned}$$

$$\begin{aligned}
 & + \|\partial_{c^*} Q_a(\mathbf{v}, \mathbf{c}^*) \cdot \partial_t \mathbf{c}^* - \partial_{c^*} Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*) \cdot \partial_t \mathbf{c}^*\|_{L_p((0,T) \times \Omega)} \\
 \leq & \|\partial_v^2 Q_a\|_\infty \|\mathbf{v}\|_\infty \|\partial_t \mathbf{v} - \partial_t \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} + \|\partial_v^2 Q_a\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_\infty \|\partial_t \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\
 & + \|\partial_v \partial_{c^*} Q_a\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_\infty \|\partial_t \mathbf{c}^*\|_{L_p((0,T) \times \Omega)} \\
 \leq & C(T_0) T^{1/p-1/\bar{p}} \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)};
 \end{aligned}$$

for the second-order spatial derivatives,

$$\begin{aligned}
 & \|\nabla^2 Q_a(\mathbf{v}, \mathbf{c}^*) - \nabla^2 Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 \leq & \|\partial_v^2 Q_a(\mathbf{v}, \mathbf{c}^*) : (\nabla \mathbf{v} \otimes \nabla \mathbf{v}) - \partial_v^2 Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*) : (\nabla \tilde{\mathbf{v}} \otimes \nabla \tilde{\mathbf{v}})\|_{L_p((0,T) \times \Omega)} \\
 & + 2\|\partial_v \partial_{c^*} Q_a(\mathbf{v}, \mathbf{c}^*) : (\nabla \mathbf{v} \otimes \nabla \mathbf{c}^*) - \partial_v \partial_{c^*} Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*) : (\nabla \tilde{\mathbf{v}} \otimes \nabla \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 & + \|\partial_{c^*}^2 Q_a(\mathbf{v}, \mathbf{c}^*) : (\nabla \mathbf{c}^* \otimes \nabla \mathbf{c}^*) - \partial_{c^*}^2 Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*) : (\nabla \mathbf{c}^* \otimes \nabla \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 \leq & \|\partial_v^2 Q_a(\mathbf{v}, \mathbf{c}^*) : (\nabla \mathbf{v} \otimes \nabla \mathbf{v} - \nabla \tilde{\mathbf{v}} \otimes \nabla \tilde{\mathbf{v}})\|_{L_p((0,T) \times \Omega)} + \\
 & \|(\partial_v^2 Q_a(\mathbf{v}, \mathbf{c}^*) - \partial_v^2 Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*)) : (\nabla \tilde{\mathbf{v}} \otimes \nabla \tilde{\mathbf{v}})\|_{L_p((0,T) \times \Omega)} \\
 & + 2\|\partial_v \partial_{c^*} Q_a(\mathbf{v}, \mathbf{c}^*) : ((\nabla \mathbf{v} - \nabla \tilde{\mathbf{v}}) \otimes \nabla \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 & + 2\|(\partial_v \partial_{c^*} Q_a(\mathbf{v}, \mathbf{c}^*) - \partial_v \partial_{c^*} Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*)) : (\nabla \tilde{\mathbf{v}} \otimes \nabla \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 & + \|(\partial_{c^*}^2 Q_a(\mathbf{v}, \mathbf{c}^*) - \partial_{c^*}^2 Q_a(\tilde{\mathbf{v}}, \mathbf{c}^*)) : (\nabla \mathbf{c}^* \otimes \nabla \mathbf{c}^*)\|_{L_p((0,T) \times \Omega)} \\
 \leq & \|\partial_v^2 Q_a\|_\infty (\|\nabla \mathbf{v}\|_\infty + \|\nabla \tilde{\mathbf{v}}\|_\infty) \|\nabla \mathbf{v} - \nabla \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} + \\
 & \|\partial_v^3 Q_a\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_\infty \|\nabla \tilde{\mathbf{v}}\|_{L_{2p}((0,T) \times \Omega)}^2 \\
 & + 2\|\partial_v \partial_{c^*} Q_a\|_\infty \|\nabla \mathbf{v} - \nabla \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \|\nabla \mathbf{c}^*\|_\infty \\
 & + 2\|\partial_v^2 \partial_{c^*} Q_a\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_\infty \|\nabla \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \|\nabla \mathbf{c}^*\|_\infty \\
 & + \|\partial_v \partial_{c^*}^2 Q_a\|_\infty \|\nabla \mathbf{v} - \nabla \tilde{\mathbf{v}}\|_\infty \|\nabla \mathbf{c}^*\|_{L_{2p}((0,T) \times \Omega)}^2 \\
 \leq & 2C^{**} \|\partial_v^2 Q_a\|_\infty (T|\Omega|)^{1/2p} \rho \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)} \\
 & + C^{**} \|\partial_v^3 Q_a\|_\infty (T|\Omega|)^{1/2p} \rho^2 \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)} \\
 & + 2C^{**} \|\partial_v \partial_{c^*} Q_a\|_\infty (T|\Omega|)^{1/2p} \|\nabla \mathbf{c}^*\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_{L_p((0,T) \times \Omega)} \\
 & + 2\|\partial_v^2 \partial_{c^*} Q_a\|_\infty (T|\Omega|)^{3/2p} \rho \|\nabla \mathbf{c}^*\|_\infty \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)} \\
 & + C^{**} \|\partial_v \partial_{c^*}^2 Q_a\|_\infty \|\nabla \mathbf{c}^*\|_{L_{2p}((0,T) \times \Omega)}^2 \|\mathbf{v} - \tilde{\mathbf{v}}\|_{W_p^{(1,2)}((0,T) \times \Omega)},
 \end{aligned}$$

where $C^{**} = C^{**}(T_0) > 0$ is a common constant for the continuous embeddings $\dot{W}_p^{(1,2)}((0, T] \times \bar{\Omega}) \hookrightarrow C([0, T]; C^1(\bar{\Omega}))$ and $\dot{W}_p^{(1,2)}((0, T] \times \bar{\Omega}) \hookrightarrow L_{2p}((0, T); W_{2p}^1(\Omega))$ with $T \in (0, T_0]$. Standard arguments now give that for suitable choice of $\rho \in (0, \rho_1]$, $T \in (0, T_1]$ (for some $\rho_1 \in (0, \rho_0]$ and $T_1 \in (0, T_0]$), the map Φ is a strictly contractive mapping from $D_{\rho, T}$ into $D_{\rho, T}$ (here, $\Phi(D_{\rho, T}) \subseteq D_{\rho, T}$ as $\mathbf{0} \in D_{\rho, T}$), thus by the strict contraction principle admits a unique fixed point $\mathbf{v}^{\text{fix}} =$

$\Phi(\mathbf{v}^{\text{fix}}) \in \mathring{W}_p^{(1,2)}((0, T] \times \overline{\Omega})$. Then, $\mathbf{c} := \mathbf{c}^* + \mathbf{v}^{\text{fix}}$ is the unique solution of the fast sorption and fast surface chemistry limit reaction diffusion system. Here, the uniqueness is valid first only in the class $\mathbf{c} \in \mathbf{c}^* + \mathbf{D}_{\rho, T}$, then arguing by contradiction shows that \mathbf{c} is actually unique in the class $\mathbf{c} \in W_p^{(1,2)}((0, T) \times \Omega; \mathbb{R}^N)$.

Moreover, for $\mathbf{c}^{*,0} \in I_p^\eta(\Omega), \eta > 0$ sufficiently small and initial values $\mathbf{c}^0 \in B_\eta(\mathbf{c}^{*,0}) \subseteq I_p^\eta(\Omega)$ close to $\mathbf{c}^{*,0}$, there is a common choice of parameters ρ_0 and T_2 to make the respective maps $\Phi = \Phi^{\mathbf{c}^0}$ strictly contractive self-mappings for any $\rho \in (0, \rho_0]$ and $T \in (0, T_2]$, so that for all these initial values the solution exists and is unique at least on the time interval $(0, T_2)$. Also it can be seen that as the maps $\Phi^{\mathbf{c}^0}$ continuously depend on the initial values, so do the fixed points, hence the solutions to the fast sorption and fast surface chemistry reaction–diffusion-limit system. □

From the proof we may extract blow-up criteria for solutions which are not global in time.

Corollary 4.9 (Blow-up criterion). *Either $T_{\max} = \infty$ (global existence), or $T_{\max} < \infty$ and $\|\mathbf{c}(t)\|_{W_p^{2-2/p}(\Omega; \mathbb{R}^N)} \rightarrow \infty$ (blow-up) or $\min_{z \in \overline{\Omega}} c_i(t, z) \rightarrow 0$ (degeneration) for some $i \in \{1, \dots, N\}$ as $t \rightarrow T_{\max}$.*

Remark 4.10. The inclusion of the case $\min c_i(t, z) \rightarrow 0$ for some i is due to the chosen linearisation around the reference function. To have enough regularity for $\mathbf{C} = \text{diag}(\mathbf{c}|_\Sigma)^{-1}$, one needs uniform positivity of the solution candidate \mathbf{c} , thus on the initial value \mathbf{c}^0 . Therefore, this approach breaks down as $\min c_i(t, \cdot) \rightarrow 0$.

4.2.2. Local-in-time existence of classical solutions in Hölder class

Analogous to the case of strong $W_p^{(1,2)}$ -solutions, we may also deduce existence of local-in-time classical solutions in the Hölder class

$$\mathbf{c} \in C^{(1,2) \cdot (1+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^N) = C^{1+\alpha}([0, T]; C(\overline{\Omega}; \mathbb{R}^N)) \cap L_\infty([0, T]; C^{2+2\alpha}(\overline{\Omega}); \mathbb{R}^N).$$

Theorem 4.11 (Local-in-time existence of classical solutions in Hölder class). *Let $\alpha \in (0, 1/2)$ and $\Omega \subseteq \mathbb{R}^n$ be a bounded domain of class $\partial\Omega \in C^{2+2\alpha}$. Then, the fast sorption and fast surface chemistry limit problem (5') admits a unique classical solution in the Hölder class $C^{(1,2) \cdot (1+\alpha)}$, if*

$$\mathbf{c}^0 \in I_\alpha^+(\overline{\Omega}) := \left\{ \mathbf{c}^0 \in C^{2+2\alpha}(\overline{\Omega}; (0, \infty)^N) : \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^0|_\Sigma \rangle = 0, \mathbf{c}^0|_\Sigma^{\Sigma, a} = \exp(-\langle \mathbf{v}^{\Sigma, a}, \boldsymbol{\mu}^0(\vartheta) \rangle) \right\}.$$

More precisely, for every reference initial value $\mathbf{c}_0^{\text{ref}} \in I_\alpha^+(\overline{\Omega})$, there are $T > 0, \varepsilon > 0$ and $C > 0$ such that the following statements hold true:

- (1) For all $\mathbf{c}^0 \in I_\alpha^+(\overline{\Omega})$ with $\|\mathbf{c}_0 - \mathbf{c}_0^{\text{ref}}\|_{I_\alpha(\overline{\Omega})} < \varepsilon$, there is a unique classical solution in the Hölder class $\mathbf{c} \in C^{(1,2) \cdot (1+\alpha)}(J \times \overline{\Omega}; (0, \infty)^N)$ of (5') for $J = [0, T]$.

(2) For any two initial values $\mathbf{c}^0, \tilde{\mathbf{c}}^0 \in I_\alpha^+(\bar{\Omega})$ with $\|\mathbf{c}^0 - \mathbf{c}^{\text{ref}}\|_{C^{2+\alpha}(\bar{\Omega})}, \|\tilde{\mathbf{c}}^0 - \mathbf{c}^{\text{ref}}\|_{C^{2+\alpha}(\bar{\Omega})} < \varepsilon$ and corresponding classical solutions $\mathbf{c}, \tilde{\mathbf{c}} \in C^{(1,2)\cdot(1+\alpha)}(J \times \bar{\Omega}; \mathbb{R}^N)$ one has

$$\|\mathbf{c} - \tilde{\mathbf{c}}\|_{C^{(1,2)\cdot(1+\alpha)}(J \times \bar{\Omega})} \leq C \|\mathbf{c}^0 - \tilde{\mathbf{c}}^0\|_{C^{2+2\alpha}(\bar{\Omega})}.$$

(3) Any (Hölder) classical solution $\mathbf{c} \in C^{(1,2)\cdot(1+\alpha)}(J \times \bar{\Omega})$ can be extended in a unique way to a maximal (Hölder) classical solution $\mathbf{c} : [0, T_{\max}) \times \Omega \rightarrow (0, \infty)^N$ (with $T_{\max} \in (0, \infty]$) with $\mathbf{c} \in C^{(1,2)\cdot(1+\alpha)}((0, T) \times \Omega; (0, \infty)^N)$ for every $T \in (0, T_{\max})$.

Proof. We may proceed as in the case of strong $W_p^{(1,2)}$ -solutions and consider a reference function $\mathbf{c}^{\text{ref}} \in C^{2+2\alpha}(\bar{\Omega})$ and $\varepsilon > 0$ such that $0 < 2\varepsilon \leq \mathbf{c}^{\text{ref}}$ on $\bar{\Omega}$. Choosing $\mathbf{c}^0 \in C^{2+2\alpha}(\bar{\Omega})$ with $\|\mathbf{c}^0 - \mathbf{c}^{\text{ref}}\|_{C^{2+2\alpha}} \leq \varepsilon$ thus implies that $\mathbf{c}^0 \geq \varepsilon$ on $\bar{\Omega}$. Now, let $\mathcal{T}(\cdot)$ denote the strongly continuous semigroup on $C^{2\alpha}(\mathbb{R}^n)$ generated by the operator $A = \mathbf{D}\Delta$ with $D(A) = C^{2+2\alpha}(\mathbb{R}^n)$, and set

$$\mathbf{c}^*(t, \cdot) = \mathcal{T}(t)\mathcal{E}\mathbf{c}^0 + \int_0^t \mathcal{T}(t-s)\mathcal{E}\mathbf{r}(\mathbf{c}^0) ds, \quad t \geq 0,$$

where $\mathcal{E} \in \mathcal{B}(C^{2+2\alpha}(\bar{\Omega}); C^{2+2\alpha}(\mathbb{R}^n)) \cap \mathcal{B}(C(\bar{\Omega}); C(\mathbb{R}^n))$ is any bounded, linear extension operator (which exists as $\partial\Omega \in C^{2+2\alpha}$). Then, $\mathcal{E}\mathbf{c}^0, \mathcal{E}\mathbf{r}(\mathbf{c}^0) \in C^{2+2\alpha}(\mathbb{R}^n) = D(A)$, hence, $\mathbf{c}^* \in C(\mathbb{R}_+; C^{2+2\alpha}(\mathbb{R}^n)) \cap C^1(\mathbb{R}_+; C^{2\alpha}(\mathbb{R}^n))$. Moreover, by maximal Hölder regularity [14, Theorem VII.10.3], it follows from $\mathbf{r}(\mathcal{E}\mathbf{c}^0) \in C^{(1,2)\cdot\alpha}(\mathbb{R}_+ \times \mathbb{R}^n)$ that, actually, $\mathbf{c}^* \in C^{(1,2)\cdot(1+\alpha)}([0, T] \times \mathbb{R}^n)$ for every $T > 0$. By the classical maximum principle (and suitable choice of \mathcal{E}) we may find $T_0 > 0$ such that $\mathbf{c}^* \geq \frac{\varepsilon}{2}$ on $[0, T_0]$, for every initial value \mathbf{c}^0 with $\|\mathbf{c}^0 - \mathbf{c}^{\text{ref}}\|_{C^{2+2\alpha}} \leq \varepsilon$.

Let us fix $\rho_0 \leq \varepsilon/(3\|\mathcal{E}\|_{\mathcal{B}(C(\bar{\Omega}); C(\mathbb{R}^n))})$ and $T_0 > 0$ as above. Then, for every $\mathbf{c}^0 \in I_\alpha^+(\bar{\Omega})$ with $\|\mathbf{c}^0 - \mathbf{c}^*\|_{C^{2+2\alpha}} \leq \varepsilon$, a function $\mathbf{c} \in C^{(1,2)\cdot(1+\alpha)}([0, T] \times \bar{\Omega})$ is a classical solution to the reaction–diffusion–sorption problem

$$\begin{aligned} \partial_t \mathbf{c} - \mathbf{D}\Delta \mathbf{c} &= \mathbf{r}(\mathbf{c}) && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c} \rangle &= 0 && \text{on } (0, T) \times \Sigma, \\ (\mathbf{c})^{v^{\Sigma, a}} &= \kappa && \text{on } (0, T) \times \Sigma, \\ \mathbf{c}(0, \cdot) &= \mathbf{c}^0 && \text{in } \Omega, \end{aligned}$$

if and only if the difference function $\mathbf{v} := \mathbf{c} - \mathbf{c}^*$ solves the semilinear parabolic system

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D}\Delta \mathbf{v} &= \mathbf{r}(\mathbf{c}^* + \mathbf{v}) - \mathbf{r}(\mathbf{c}^0) && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{v}|_\Sigma \rangle &= \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^*|_\Sigma \rangle && \text{on } (0, T) \times \Sigma, \\ \mathbf{C}_a^* \mathbf{v}^\Sigma &= \kappa_a - (\mathbf{c}^*)^{v^{\Sigma, a}} - \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) && \text{on } (0, T) \times \Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{0} && \text{in } \Omega \end{aligned}$$

with \mathcal{Q}_a defined as in the local-in-time existence proof for strong $W_p^{(1,2)}$ -solutions. We remark that $\mathcal{Q}(\mathbf{v}, \mathbf{c}^*)|_{t=0} = \mathcal{Q}_a(\mathbf{0}, \mathbf{c}^0) = \mathbf{0}$, $\mathbf{r}(\mathbf{c}^*)|_{t=0} = \mathbf{r}(\mathbf{c}^0)$ as well as $\kappa_a - (\mathbf{c}^*)^{\nu^{\Sigma,a}}|_{\{0\} \times \Sigma} = \kappa_a - (\mathbf{c}^0)^{\nu^{\Sigma,a}}|_{\Sigma} = 0$ and $\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^*|_{\{0\} \times \Sigma} \rangle = \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^0|_{\Sigma} \rangle = 0$. This allows to seek for \mathbf{v} as a fixed point of the map

$$\Phi : \mathbf{D}_{\rho,T} := \left\{ \mathbf{v} \in C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega}) : \right. \\ \left. \mathbf{v}|_{t=0} = \mathbf{0}, \|\mathbf{v}\|_{C^{(1,2)\cdot(1+\alpha)}} \leq \rho \right\} \rightarrow C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega})$$

defined by $\Phi(\mathbf{v}) := \mathbf{w}$, where \mathbf{w} is the classical solution to the quasi-autonomous problem

$$\begin{aligned} \partial_t \mathbf{w} - \mathbf{D}\Delta \mathbf{w} &= \mathbf{r}(\mathbf{c}^* + \mathbf{v}) - \mathbf{r}(\mathbf{c}^0) && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{w}|_{\Sigma} \rangle &= \langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{c}^*|_{\Sigma} \rangle && \text{on } (0, T) \times \Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{w}|_{\Sigma} \rangle &= \kappa_a - (\mathbf{c}^*)^{\nu^{\Sigma,a}} - \mathcal{Q}_a(\mathbf{v}, \mathbf{c}^*) && \text{on } (0, T) \times \Sigma, \\ \mathbf{w}(0, \cdot) &= \mathbf{0}. \end{aligned}$$

We may now proceed as for the case of strong solutions, one helpful result being the auxiliary Lemma 4.12.

Details are left to the reader. □

Let us write

$$\begin{aligned} \mathring{C}^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^N) &= \left\{ \mathbf{v} \in C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^N) : \mathbf{v}(0, \cdot) = \mathbf{0} \right\}, \\ \mathring{C}^{(1,2)\cdot(1/2+\alpha)}((0, T] \times \overline{\Omega}; \mathbb{R}^{n^\Sigma}) &= \left\{ \mathbf{g} \in C^{(1,2)\cdot(1/2+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^{n^\Sigma}) : \mathbf{g}(0, \cdot) = \mathbf{0} \right\}. \end{aligned}$$

Lemma 4.12 (Locally uniform maximal regularity constant). *Let $\alpha > 0$ and $\Omega \subseteq \mathbb{R}^n$ be a bounded domain of class $\partial\Omega \in C^{2+2\alpha}$. Moreover, let $T_0 > 0$ and $\mathbf{c}^* \in C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^N)$ with $\mathbf{c}^* \geq \varepsilon > 0$ be given. Then, there is a constant $C = C(T_0, \varepsilon, \|\mathbf{c}^*\|_{C^{(1,2)\cdot(1+\alpha)}}) > 0$ such that for every $T \in (0, T_0]$ and every $\mathbf{f} \in C^{(1,2)\cdot\alpha}([0, T] \times \overline{\Omega}; \mathbb{R}^N)$, $\mathbf{g} \in \mathring{C}^{(1,2)\cdot(1/2+\alpha)}((0, T] \times \overline{\Omega}; \mathbb{R}^{n^\Sigma})$ there is a unique solution $\mathbf{v} \in \mathring{C}^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega}; \mathbb{R}^N)$ of the linear parabolic initial-boundary value problem*

$$\begin{aligned} \partial_t \mathbf{v} - \mathbf{D}\Delta \mathbf{v} &= \mathbf{f} && \text{in } (0, T) \times \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D}\partial_n \mathbf{v}|_{\Sigma} \rangle &= g_k && \text{on } (0, T) \times \Sigma, \\ \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma,a}, \mathbf{v}|_{\Sigma} \rangle &= h_a && \text{on } (0, T) \times \Sigma, \\ \mathbf{v}(0, \cdot) &= \mathbf{0} && \text{in } \Omega \end{aligned}$$

and it holds the estimate

$$\begin{aligned} \|\mathbf{v}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega})} &\leq C \left(\|\mathbf{f}\|_{C^{(1,2)\cdot\alpha}([0, T] \times \overline{\Omega})} + \|\mathbf{g}\|_{C^{(1,2)\cdot(1/2+\alpha)}([0, T] \times \Sigma)} \right. \\ &\quad \left. + \|\mathbf{h}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T] \times \overline{\Omega})} \right). \end{aligned}$$

Proof. As demonstrated (for the half-space case) in Proposition 4.2 in combination with Lemma 4.3, the Lopatinskiĭ–Shapiro condition is satisfied, so that Hölder-maximal regularity follows by [14, Theorem VIII.10.4] (where for nonzero initial values complying with the compatibility condition, the maximal regularity constant may, in general, depend on $T \in (0, T_0]$ as well). Let us demonstrate that for zero initial values, the maximal regularity constant may be chosen uniformly for $T \in (0, T_0]$. To see this, let $\chi \in C^\infty(\mathbb{R})$ be any function such that $\chi \equiv 1$ on $(-\infty, \frac{4}{3}]$ and $\chi \equiv 0$ on $[5/3, \infty)$, say. Given any $T \in (0, T_0]$, and $\mathbf{f}, \mathbf{g}, \mathbf{h}$ as in the statement of the theorem, we may now extend these functions by setting

$$\begin{cases} \vec{f}(t, x) = \begin{cases} \vec{f}(t, x), & t \in [0, T], x \in \Omega, \\ \vec{f}(2T - t, x), & t \in (T, 2T], x \in \Omega, \\ \vec{0}, & t > 2T, x \in \Omega, \end{cases} \\ \vec{g}(t, x) = \begin{cases} \vec{g}(t, x), & t \in [0, T], x \in \Sigma, \\ \vec{g}(2T - t, x), & t \in (T, 2T], x \in \Sigma, \\ \vec{0}, & t > 2T, x \in \Sigma, \end{cases} \\ \vec{h}(t, x) = \begin{cases} \vec{h}(t, x), & t \in [0, T], x \in \Sigma, \\ 2\xi \left(\frac{t-T}{T}\right) \vec{h}(T, x) - \vec{h}(2T - t, x), & t \in (T, 2T], x \in \Sigma, \\ \vec{0}, & t > 2T, x \in \Sigma. \end{cases} \end{cases}$$

Then, for $\alpha \in (0, 1/2]$ one easily deduces that $\vec{f} \in C^{(1,2)\text{-}\alpha}(\mathbb{R}_+ \times \bar{\Omega}; \mathbb{R}^N)$ and $\vec{g} \in C^{(1,2)\text{-}(1/2+\alpha)}(\mathbb{R}_+ \times \bar{\Omega}; \mathbb{R}^{n_\Sigma})$ with norms

$$\begin{aligned} \|\vec{f}\|_{C^{(1,2)\text{-}\alpha}(\mathbb{R}_+ \times \bar{\Omega})} &= \|\mathbf{f}\|_{C^{(1,2)\text{-}\alpha}([0, T] \times \bar{\Omega})}, \\ \|\vec{g}\|_{C^{(1,2)\text{-}(1/2+\alpha)}(\mathbb{R}_+ \times \bar{\Omega})} &= \|\mathbf{g}\|_{C^{(1,2)\text{-}(1/2+\alpha)}([0, T] \times \bar{\Omega})}. \end{aligned}$$

For \vec{h} , we obtain that

$$\begin{aligned} \|\vec{h}(t, \cdot)\|_{C^{2+2\alpha}(\Sigma)} &\leq 3\|\chi\|_\infty \|\mathbf{h}\|_{C([0, T]; C^{2+2\alpha}(\Sigma))} \quad \text{for every } t \geq 0, \\ \|\partial_t \vec{h}(t, \cdot)\|_\infty &\leq 3\|\chi\|_\infty \|\partial_t \mathbf{h}\|_\infty + \sup_{\tau \in [T, 2T]} \left\| \frac{2}{T} \chi' \left(\frac{\tau-T}{T}\right) \mathbf{h}(T, \cdot) \right\|_\infty \\ &\leq 3\|\chi\|_\infty \|\partial_t \mathbf{h}\|_\infty + \frac{2}{T} \|\chi'\|_\infty \int_0^T \|\partial_t \mathbf{h}(\tau, \cdot)\|_\infty \, d\tau \\ &\leq 3\|\chi\|_\infty \|\partial_t \mathbf{h}\|_\infty + \frac{2}{T} \|\chi'\|_\infty \int_0^T \tau^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \, d\tau \\ &\leq 3\|\chi\|_\infty \|\partial_t \mathbf{h}\|_\infty + \frac{2}{1+\alpha} \|\chi'\|_\infty T^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\ &\leq 3\|\chi\|_\infty \|\partial_t \mathbf{h}\|_\infty + \frac{2}{1+\alpha} \|\chi'\|_\infty T_0^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))}, \\ \|\partial_t \vec{h}(t, \cdot) - \partial_t \vec{h}(s, \cdot)\|_\infty &\leq \|\chi\|_\infty \|\partial_t \mathbf{h}(2T - t, \cdot) - \partial_t \mathbf{h}(2T - s, \cdot)\|_\infty \end{aligned}$$

$$\begin{aligned}
 & + \frac{2}{T} \left| \chi' \left(\frac{t-T}{T} \right) - \chi' \left(\frac{s-T}{T} \right) \right| \|\mathbf{h}(T, \cdot)\|_\infty \\
 & \leq \|\chi\|_\infty [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} |s - t|^\alpha \\
 & \quad + [\chi']_{C^\alpha} |s - t|^\alpha \|\mathbf{h}\|_\infty, \quad \text{for } s, t \in [T, 2T], \\
 \|\partial_t \tilde{\mathbf{h}}(t, \cdot) - \partial_t \tilde{\mathbf{h}}(s, \cdot)\|_\infty & = \left\| \frac{2}{T} \chi' \left(\frac{t-T}{T} \right) \mathbf{h}(T, \cdot) + \partial_t \mathbf{h}(2T - t, \cdot) - \partial_t \mathbf{h}(s, \cdot) \right\|_\infty \\
 & \leq \frac{2}{T} \left| \chi' \left(\frac{t-T}{T} \right) - \chi'(0) \right| \|\mathbf{h}(T, \cdot)\|_\infty \\
 & \quad + \|\chi\|_\infty \|\partial_t \mathbf{h}(2T - t, \cdot) - \partial_t \mathbf{h}(s, \cdot)\|_\infty \\
 & \leq \frac{2}{T} \left| \frac{t-T}{T} \right|^\alpha [\chi']_\alpha \int_0^T \|\partial_t \mathbf{h}(\tau, \cdot)\|_\infty d\tau \\
 & \quad + \|\chi\|_\infty |2T - t - s|^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & \leq \frac{2}{T} \left| \frac{t-T}{T} \right|^\alpha [\chi']_\alpha \int_0^T \tau^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} d\tau \\
 & \quad + \|\chi\|_\infty |2T - t - s|^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & = \frac{2}{1 + \alpha} |t - T|^\alpha [\chi']_\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & \quad + \|\chi\|_\infty |2T - t - s|^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & \leq \frac{2}{1 + \alpha} |t - s|^\alpha [\chi']_\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & \quad + \|\chi\|_\infty |t - s|^\alpha [\partial_t \mathbf{h}]_{C^\alpha([0, T]; C(\Sigma))} \\
 & \quad \text{for } 0 \leq s \leq T \leq t \leq 2T.
 \end{aligned}$$

Therefore, there is a constant $C = C(\alpha)$, independent of $T \in (0, T_0]$ and $T_0 > 0$ such that

$$\|\tilde{\mathbf{h}}\|_{C^{(1,2)\cdot(1+\alpha)}(\mathbb{R}_+ \times \Sigma)} \leq C \|\mathbf{h}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T] \times \Sigma)}.$$

We may therefore consider $\mathbf{v} = \tilde{\mathbf{v}}|_{[0, T] \times \bar{\Omega}}$ as the restriction to time $t \in [0, T]$ of the solution of the parabolic initial-boundary value problem on $(0, T_0)$

$$\begin{aligned}
 \partial_t \tilde{\mathbf{v}} - \mathbf{D} \Delta \tilde{\mathbf{v}} &= \tilde{\mathbf{f}} && \text{in } (0, T) \times \Omega, \\
 -\langle \mathbf{e}^k, \mathbf{D} \partial_n \tilde{\mathbf{v}} \rangle &= \tilde{g}_k && \text{on } (0, T) \times \Sigma, \\
 \langle \mathbf{C}_a^* \mathbf{v}^{\Sigma, a}, \tilde{\mathbf{v}} \rangle &= \tilde{h}_a && \text{on } (0, T) \times \Sigma, \\
 \tilde{\mathbf{v}}(0, \cdot) &= \mathbf{0} && \text{in } \Omega,
 \end{aligned}$$

and may deduce that

$$\begin{aligned}
 \|\mathbf{v}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T] \times \bar{\Omega})} & \leq \|\tilde{\mathbf{v}}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T_0] \times \bar{\Omega})} \\
 & \leq C(T_0) \left(\|\tilde{\mathbf{f}}\|_{C^{(1,2)\cdot\alpha}([0, T_0] \times \Omega)} + \|\tilde{\mathbf{g}}\|_{C^{(1,2)\cdot(1/2+\alpha)}([0, T_0] \times \Sigma)} + \|\tilde{\mathbf{h}}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T_0] \times \bar{\Omega})} \right) \\
 & \leq C(T_0) \left(\|\mathbf{f}\|_{C^{(1,2)\cdot\alpha}([0, T] \times \Omega)} + \|\mathbf{g}\|_{C^{(1,2)\cdot(1/2+\alpha)}([0, T] \times \Sigma)} + \|\mathbf{h}\|_{C^{(1,2)\cdot(1+\alpha)}([0, T] \times \bar{\Omega})} \right).
 \end{aligned}$$

□

4.2.3. *A priori bounds on the strong solution of the fast sorption and fast surface chemistry model*

In the previous subsection, it has been noticed that a bound on the phase space norm $\| \cdot \|_{W_p^{2-2/p}}$ is enough for establishing global existence of a strong solution. To derive such a bound, however, is a delicate matter, and it is not clear whether global existence holds true in all cases. On the other hand, for some weaker norms at least a priori bounds can be established *for free*. The derivation of these a priori bounds is based on the parabolic maximum principle and entropy considerations, highlighting the fruitful interplay between mathematics and physics, and will be presented in this subsection.

Theorem 4.13 (A priori bounds). *Let $\mathbf{c}^0 \in I_p^+(\Omega) \cap C^2(\overline{\Omega}; \mathbb{R}^N)$ and $\mathbf{c} \in C^{(1,2)}([0, T_{\max}) \times \overline{\Omega}; \mathbb{R}_+^N)$ be a maximal classical solution to the fast sorption and fast surface chemistry limit problem*

$$\begin{aligned} \partial_t \mathbf{c} - \mathbf{D} \Delta \mathbf{c} &= \mathbf{r}(\mathbf{c}), & t \geq 0, \quad \mathbf{z} \in \Omega, \\ -\langle \mathbf{e}^k, \mathbf{D} \partial_n \mathbf{c} \rangle &= \mathbf{0}, & t \geq 0, \quad \mathbf{z} \in \Sigma, \quad k = 1, \dots, n^\Sigma, \\ k_a^f \mathbf{c}^{\alpha^{\Sigma,a}} &= k_a^b \mathbf{c}^{\beta^{\Sigma,a}} & t \geq 0, \quad \mathbf{z} \in \Sigma, \quad a = 1, \dots, m^\Sigma, \\ \mathbf{c}(0, \cdot) &= \mathbf{c}^0, & \mathbf{z} \in \overline{\Omega}. \end{aligned}$$

Further, assume that there is a conserved quantity with strictly positive entries, i.e. there is

$$\mathbf{e} \in (0, \infty)^N \cap \{ \mathbf{v}^a : a = 1, \dots, m \}^\perp \cap \{ \mathbf{v}^{\Sigma,a} : a = 1, \dots, m^\Sigma \}^\perp.$$

Then, for every $T_0 \in (0, T_{\max}] \cap \mathbb{R}$ there is $C = C(T_0) > 0$, also depending on the initial value \mathbf{c}^0 , such that the following a priori bounds hold true:

- (1) $L^\infty L^1$ —a priori estimate:

$$\sup_{t \in [0, T_0]} \| \mathbf{c}(t, \cdot) \|_{L^1(\Omega; \mathbb{R}^N)} \leq C \| \mathbf{c}^0 \|_{L^1(\Omega; \mathbb{R}^N)},$$

where the constant can actually be chosen independently of \mathbf{c}^0 and T_0 , but only depends on the ratio between the smallest and largest entry of $\mathbf{e} \in (0, \infty)^N$;

- (2) $L^1 L^\infty$ —a priori estimate:

$$\sup_{\mathbf{z} \in \overline{\Omega}} \| \mathbf{c}(\cdot, \mathbf{z}) \|_{L^1([0, T_0]; \mathbb{R}^N)} \leq C;$$

- (3) $L^2 L^2$ —a priori estimate:

$$\| \mathbf{c} \|_{L^2([0, T_0] \times \Omega; \mathbb{R}^N)} \leq C;$$

- (4) Moreover, provided the surface chemistry is constructed from thermodynamic principles, i.e. the affinity $\mathcal{A}_a = \mu_i^\Sigma v_i^\Sigma$ vanishes for chemical equilibria, and

$\mu_i^\Sigma = \mu_i|_\Sigma = \mu_i^0 + \ln c_i|_\Sigma$ for equilibria for adsorption and desorption, the following entropy identity holds true:

$$\begin{aligned} & \int_\Omega c_i(t, \mathbf{z})(\mu_i^0 + \ln c_i(t, \mathbf{z}) - 1) \, d\mathbf{z} \\ & + \int_0^t \int_\Omega \sum_{i=1}^N d_i \frac{|\nabla c_i(s, \mathbf{z})|^2}{c_i(s, \mathbf{z})} \, d\mathbf{z} \, ds + \sum_{a=1}^m \int_0^t \int_\Omega \left(\sum_{i=1}^N \ln(c_i) v_i^a \right) \\ & \quad \left(\exp \left(\sum_{i=1}^N \ln(c_i) v_i^a \right) - 1 \right) \, d\mathbf{z} \, ds \\ & = \int_\Omega c_i^0(\mathbf{z})(\mu_i^0 \ln c_i^0(\mathbf{z}) - 1) \, d\mathbf{z}, \quad t \in [0, T_0]. \end{aligned}$$

Proof. $L^\infty L^1$ -a priori estimate: Since $\mathbf{e} \in (0, \infty)^N$ is a conserved quantity for both the bulk and surface chemistry, $\langle \mathbf{r}(\mathbf{c}), \mathbf{e} \rangle = \langle \mathbf{r}^\Sigma(\mathbf{c}), \mathbf{e} \rangle = 0$ for all values of \mathbf{c} , where $\mathbf{r}^\Sigma(\mathbf{c}) = k_a^f \mathbf{c}^{\alpha^{\Sigma,a}} - k_a^b \mathbf{c}^{\beta^{\Sigma,a}}$. Thus, using regularity properties of parameter-dependent integrals and the divergence theorem, for every $t \in [0, T_0]$ it holds that

$$\begin{aligned} \frac{d}{dt} \int_\Omega \langle \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} &= \int_\Omega \langle \partial_t \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} = \int_\Omega \langle \mathbf{D} \Delta \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} + \int_\Omega \langle \mathbf{r}(\mathbf{c}(t, \mathbf{z})), \mathbf{e} \rangle \, d\mathbf{z} \\ &= \int_\Omega \langle \mathbf{D} \Delta \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} = \int_{\partial\Omega} \langle \mathbf{D} \partial_n \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\sigma(\mathbf{z}) = 0. \end{aligned}$$

As a result,

$$\int_\Omega \langle \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} = \int_\Omega \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z}, \quad t \in [0, T_0]$$

and, since $\mathbf{e} \in (0, \infty)^N$, the map $c \mapsto \int_\Omega \sum_{i=1}^N |c_i(\mathbf{z})| e_i \, d\mathbf{z}$ defines a norm which is equivalent to the standard L_1 -norm on the Lebesgue space $L_1(\Omega; \mathbb{R}^N)$. More precisely,

$$\|\mathbf{c}(t, \cdot)\|_{L_1(\Omega; \mathbb{R}^N)} \leq \frac{1}{\min_i e_i} \int_\Omega \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} \leq \frac{\max_i e_i}{\min_i e_i} \|\mathbf{c}^0\|_{L_1(\Omega; \mathbb{R}^N)},$$

establishing the first a priori estimate with

$$C = \frac{\max_i e_i}{\min_i e_i}$$

independent of $T_0 > 0$ and the initial value \mathbf{c}^0 .

$L^1 L^\infty$ -a priori estimate: To derive the $L_1 L^\infty$ -a priori bound, let us consider the function $w : [0, T_0) \times \bar{\Omega} \rightarrow [0, \infty)$ defined by

$$w(t, \mathbf{z}) = \int_0^t \langle \mathbf{D} \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle \, ds, \quad t \in [0, T_0), \mathbf{z} \in \bar{\Omega}.$$

As a parameter integral of a $C^{(1,2)}$ -function, w has the regularity $w \in C^2([0, T_0) \times \bar{\Omega})$ and using elementary results on parameter-dependent integrals, the evolution (5) and the assumption that \mathbf{e} is a conserved quantity, we establish the estimate

$$\partial_t w(t, \mathbf{z}) = \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \leq d_{\max} \langle \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle$$

$$\begin{aligned}
 &= d_{\max} \left(\int_0^t \langle \partial_t \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds + \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \right) \\
 &= d_{\max} \left(\int_0^t \langle \mathbf{D} \Delta \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle + \langle \mathbf{r}(\mathbf{c}(s, \mathbf{z})), \mathbf{e} \rangle ds + \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \right) \\
 &= d_{\max} \left(\int_0^t \langle \mathbf{D} \Delta \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds + \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \right) \\
 &= d_{\max} \left(\Delta w(t, \mathbf{z}) + d_{\max} \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \right), \quad t \in [0, T_0), \quad \mathbf{z} \in \Omega \\
 \partial_n w(t, \mathbf{z}) &= \int_0^t \langle \mathbf{D} \partial_n \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds = 0, \quad t \in [0, T_0), \quad \mathbf{z} \in \partial \Omega \\
 w(0, \mathbf{z}) &= 0, \quad \mathbf{z} \in \bar{\Omega}.
 \end{aligned}$$

Therefore, $w \geq 0$ satisfies the system of differential inequalities

$$\begin{aligned}
 \partial_t w - d_{\max} \Delta w &\leq d_{\max} \langle \mathbf{c}^0, \mathbf{e} \rangle, \quad t \in [0, T_0), \quad \mathbf{z} \in \Omega \\
 \partial_n w &= 0, \quad t \in [0, T_0), \quad \mathbf{z} \in \partial \Omega \\
 w(0, \mathbf{z}) &= 0, \quad \mathbf{z} \in \bar{\Omega}.
 \end{aligned}$$

From the parabolic maximum principle for differential inequalities, it then follows that there is $C > 0$ (depending on T_0 and \mathbf{c}^0) such that

$$0 \leq w(t, \mathbf{z}) \leq C, \quad t \in [0, T_0), \quad \mathbf{z} \in \Omega$$

and, consequently, one finds that

$$\| \mathbf{c}(\cdot, \mathbf{z}) \|_{L_1((0, T_0); \mathbb{R}^N)} \leq C, \quad \mathbf{z} \in \Omega.$$

L₂^tL₂^z--a priori estimate: For the L₂-estimate, let us fix $T \in (0, T_0)$. Employing integration by parts, Fubini’s theorem, the no-flux boundary conditions on the conserved part and the fundamental theorem of calculus, we find for the integral

$$\begin{aligned}
 &\int_0^T \int_{\Omega} \langle \mathbf{D} \mathbf{c}, \mathbf{e} \rangle \langle \mathbf{c}, \mathbf{e} \rangle dz dt \\
 &= \int_0^T \int_{\Omega} \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \left(\Delta \int_0^t \langle \mathbf{D} \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds + \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \right) dz dt \\
 &= \int_0^T \int_{\Omega} \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \Delta \int_0^t \langle \mathbf{D} \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds dz dt \\
 &\quad + \int_0^T \int_{\Omega} \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle dz dt \\
 &= - \int_{\Omega} \int_0^T \nabla \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \cdot \nabla \int_0^t \langle \mathbf{D} \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds dt dz \\
 &\quad + \int_0^T \int_{\Sigma} \langle \mathbf{D} \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \int_0^t \langle \mathbf{D} \partial_n \mathbf{c}(s, \mathbf{z}), \mathbf{e} \rangle ds d\sigma(\mathbf{z}) dt
 \end{aligned}$$

$$\begin{aligned}
 &+ \int_0^T \int_{\Omega} \langle \mathbf{D}\mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} \, dt \\
 &= -\frac{1}{2} \int_{\Omega} \left| \int_0^T \nabla \langle \mathbf{D}\mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, dt \right|^2 \, d\mathbf{z} + \int_0^T \int_{\Omega} \langle \mathbf{D}\mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} \, dt \\
 &\leq \int_0^T \int_{\Omega} \langle \mathbf{D}\mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} \, dt \\
 &\leq \frac{d_{\max}}{d_{\min}} T \|\langle \mathbf{c}^0, \mathbf{e} \rangle\|_{L^\infty(\Omega)} \|\langle \mathbf{D}\mathbf{c}^0, \mathbf{e} \rangle\|_{L^1(\Omega)}, \quad T \in (0, T_0),
 \end{aligned}$$

where in the last step it has been used that $\mathbf{c} \geq \mathbf{0}$ and, therefore,

$$\begin{aligned}
 \int_{\Omega} \langle \mathbf{D}\mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} &\leq d_{\max} \int_{\Omega} \langle \mathbf{c}(t, \mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} = d_{\max} \int_{\Omega} \langle \mathbf{c}^0(\mathbf{z}), \mathbf{e} \rangle \, d\mathbf{z} \\
 &\leq \frac{d_{\max}}{d_{\min}} \int_{\Omega} \langle \mathbf{D}\mathbf{c}^0, \mathbf{e} \rangle \, d\mathbf{z}.
 \end{aligned}$$

One may thus take

$$C = \frac{d_{\max}}{d_{\min}} T_0 \|\langle \mathbf{c}^0, \mathbf{e} \rangle\|_{L^\infty(\Omega)} \|\langle \mathbf{D}\mathbf{c}^0, \mathbf{e} \rangle\|_{L^1(\Omega)}.$$

Entropy identity: By the theorem on derivatives of parameter-dependent integrals, and as the derivative of the function $(0, \infty) \in x \mapsto x(\ln x - 1)$ is $\ln x$ for all $x \in (0, \infty)$, one finds that

$$\begin{aligned}
 &\frac{d}{dt} \int_{\Omega} \sum_i c_i (\mu_i^0 + \ln(c_i) - 1) \, d\mathbf{z} \\
 &= \int_{\Omega} \partial_t c_i (\mu_i^0 + \ln(c_i)) \, d\mathbf{z} = \int_{\Omega} \sum_i (d_i \Delta c_i + r_i(\mathbf{c})) (\mu_i^0 + \ln(c_i)) \\
 &= - \int_{\Omega} \sum_i \frac{d_i |\nabla c_i|^2}{c_i} \, d\mathbf{z} + \int_{\Sigma} \sum_i (\mu_i^0 + \ln(c_i)) d_i \partial_n c_i \, d\sigma(\mathbf{z}) \\
 &\quad + \int_{\Omega} \sum_i r_i(\mathbf{c}) (\mu_i^0 + \ln c_i) \, d\mathbf{z}
 \end{aligned}$$

The assertion will be established if $\sum_i (\mu_i^0 + \ln(c_i)) d_i \partial_n c_i \, d\sigma(\mathbf{z}) = 0$ can be proved. From the boundary conditions $\langle \mathbf{e}^k, \partial_n(\mathbf{D}\mathbf{c}) \rangle = 0$, there are scalar functions $\eta_a : [0, T_0) \times \Sigma \rightarrow \mathbb{R}$ such that $\partial_n(\mathbf{D}\mathbf{c})|_{\Sigma} = \sum_{a=1}^{m_{\Sigma}} \eta_a \mathbf{v}^{\Sigma,a}$. Hence,

$$\begin{aligned}
 \sum_i (\mu_i^0 + \ln(c_i)) d_i \partial_n c_i &= \langle \boldsymbol{\mu}^0 + \ln(\mathbf{c}), \partial_n(\mathbf{D}\mathbf{c}) \rangle \\
 &= \sum_a \eta_a \langle \boldsymbol{\mu}^0 + \ln(\mathbf{c}), \mathbf{v}^{\Sigma,a} \rangle = \sum_a \eta_a \sum_{i=1}^N (\mu_i^0 + \ln(c_i)) v_i^{\Sigma,a} \\
 &= 0
 \end{aligned}$$

by assumption since for all times $t \geq 0$ and at all positions $\vec{z} \in \Sigma$ the sorption processes and the surface chemistry are in equilibrium. Therefore, this contribution to the sum vanishes, and the entropy identity follows by the fundamental theorem of calculus. \square

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