Mathematical Analysis of Marine Ecosystem Models

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Abstract

This work is concerned with the mathematical formulation of marine ecosystem models. The understanding of marine ecosystems is of increasing importance in climate research because oceanic processes influence global biogeochemical cycles, especially the carbon cycle.

Marine ecosystem models describe the concentrations of all involved constituents (e.g. phosphate) as solutions of advection-diffusion-reaction equations. The system consisting of these equations is referred to as "the model equation". The influence of biogeochemical reactions (e.g. consumption of nutrients, growth, decomposition) is modeled by reaction terms which are, in general, nonlinear functions of all regarded concentrations. The reaction terms additionally include parameters (e.g. growth rates). The parameters may depend on space and time although they are assumed to be constant in most applications. The determination of parameter values enables the model's adjustment to the ecosystem in question, i.e., to observed concentrations. In this work, the adjustment takes place within the framework of a mathematical optimization problem (parameter identification problem).

In applications, the model equation and the parameter identification problem are solved numerically. A satisfying assessment of numerical solutions requires information about the continuous model. However, such information is practically never available. In this work, we fill this gap by investigating the continuous equation of a general ecosystem model and the corresponding parameter identification problem.

As a result, we obtain existence of transient as well as periodic solutions. In the case of transient solutions, i.e., solutions with a prescribed initial value, we investigate models characterized by a combination of monotone and Lipschitz continuous reaction terms. We prove two existence and uniqueness theorems for transient weak solutions. The proofs rely on standard methods (Galerkin's method, Banach's Fixed Point Theorem) which we adapt to the nonlinearly coupled systems of equations and the two types of reaction terms. Periodic solutions are characterized by equal initial and terminal values. We investigate periodic solutions of an important model class considering conservation of mass. This condition, which we introduce and investigate separately, effects that the constant zero function is a periodic solution. Finding a nontrivial periodic solution is a challenging task which is usually not treated in literature. The existence result we prove in this work ensures that a periodic solution exists for each prescribed mass in the ecosystem. From this it follows that there are nontrivial solutions (those corresponding to a nontrivial mass), and that periodic solutions are not unique.

Concerning parameter identification, we prove the existence of optimal parameter values for all measured concentrations which are at least quadratically integrable. The existence theorem, proved by means of an adapted standard method from optimal control theory, treats both the transient and the periodic case simultaneously and admits variable parameters. In addition, we indicate first and second order optimality conditions and formulate the first order condition as an optimality system. The technique we use to obtain the optimality system is not directly applicable in the periodic case since, in general, periodic solutions are not unique. For this reason, we investigate an auxiliary problem based on a transient instead of a periodic model equation. The newly introduced initial value is regarded as an additional parameter which is optimized in such a way that the solution of the model equation associated with the optimal parameter value is approximately periodic.

We apply all theoretical results to the PO_4-DOP model which is important for testing purposes. By means of a numerical test based on a two-dimensional version of the PO_4-DOP model, we investigate uniqueness of numerically computed periodic solutions.

Zusammenfassung

Im Fokus dieser Arbeit steht die mathematische Formulierung mariner Ökosystemmodelle. Im Bereich der Klimaforschung ist das Verständnis mariner Ökosysteme von wachsender Bedeutung, da ozeanische Prozesse globale biogeochemische Kreisläufe, insbesondere den Kohlenstoffkreislauf, beeinflussen.

Marine Ökosystemmodelle beschreiben die Konzentrationen aller zum System gehörenden Stoffe (z. B. Phosphat) als Lösungen von Advektions-Diffusions-Reaktions-Gleichungen. Das System, das aus diesen Gleichungen besteht, wird als „die Modellgleichung“ bezeichnet. Der Einfluss der biogeochemischen Reaktionen (wie etwa der Aufnahme von Nährstoffen, Wachstum, Abbau) wird mittels Reaktionstermen modelliert. Dies sind im Allgemeinen nichtlineare Funktionen aller im Modell betrachteten Konzentrationen. Die Reaktionsterme hängen zusätzlich von Parametern (z. B. Wachstumsraten) ab. Diese werden oft als konstant angenommen, können aber auch von Zeit und Ort abhängen. Die Bestimmung der Parameter ermöglicht eine Anpassung des Modells an das zu beschreibende Ökosystem, d.h. an tatsächlich gemessene Konzentrationen. In dieser Arbeit erfolgt die Anpassung im Rahmen eines mathematischen Optimierungsproblems (Parameteridentifikationsproblem).

In Anwendungen werden die Modellgleichung und das Parameteridentifikationsproblem numerisch gelöst. Eine zufriedenstellende Beurteilung numerischer Lösungen erfordert Informationen über das kontinuierliche Modell. Solche Informationen sind jedoch für kein uns bekanntes Modell verfügbar. Mit dieser Arbeit beheben wir diesen Mangel, indem wir die kontinuierliche Gleichung eines allgemeinen Modells und das zugehörige Parameteridentifikationsproblem untersuchen.

Als Ergebnis erhalten wir Existenzresultate für transiente und periodische schwache Lösungen. Im Falle transienter Lösungen, also Lösungen zu einem vorgegebenen Anfangswert, untersuchen wir Modelle, die durch eine Kombination monotoner und Lipschitz-stetiger Reaktionsterme gekennzeichnet sind. Wir beweisen zwei Aussagen zur Existenz und Eindeutigkeit transienter schwacher Lösungen. Die Beweise beruhen auf Standardmethoden, welche wir an das nichtlinear gekoppelte System partieller Differentialgleichungen und die genannten Reaktionsterme anpassen. Periodische Lösungen werden durch gleiche Anfangs- und Endwerte charakterisiert. Wir untersuchen periodische Lösungen einer wichtigen Modellklasse, bei der Massenerhaltung berücksichtigt wird. Diese Bedingung, die wir gesondert einführen und untersuchen, bewirkt, dass die konstante Nullfunktion eine periodische Lösung der Modellgleichung ist. Die Suche nach nichttrivialen periodischen Lösungen ist eine herausfordernde Aufgabenstellung, die in der Literatur gewöhnlich nicht behandelt wird. Das Existenzresultat, das wir in dieser Arbeit beweisen, sagt aus, dass es zu jeder vorgegebenen Masse im Ökosystem eine periodische Lösung gibt. Daraus folgt erstens, dass es nichttriviale periodische Lösungen gibt (nämlich jene, die zu einer nichttrivialen Masse gehören), und zweitens, dass periodische Lösungen der betrachteten Modelle nicht eindeutig sind.

Im Zusammenhang mit dem Parameteridentifikationsproblem zeigen wir die Existenz optimaler Parameterwerte zu jeder gemessenen Konzentration, die mindestens quadratintegrierbar ist. Der Existenzsatz, der mithilfe einer Standardmethode aus der Optimalsteuerungstheorie bewiesen wird, behandelt den transienten und den periodischen Fall gleichzeitig und lässt variable Parameter zu. Zusätzlich geben wir Optimalitätsbedingungen erster und zweiter Ordnung an und formulieren die Bedingung erster Ordnung als Optimalitätssystem. Die dafür verwendete Technik ist nicht unmittelbar auf den periodischen Fall anwendbar, da periodische Lösungen im Allgemeinen nicht eindeutig sind. Daher untersuchen wir in diesem Fall ein Hilfsproblem, dem eine transiente Modellgleichung zugrunde liegt. Der neu eingeführte

Anfangswert wird als zusätzlicher Parameter aufgefasst, der so optimiert wird, dass die zum optimalen Parameterwert gehörende Lösung der Modellgleichung näherungsweise periodisch ist.

Wir wenden alle theoretischen Ergebnisse auf das PO_4-DOP-Modell an, das zu Testzwecken herangezogen werden kann. Mittels eines numerischen Tests, der auf einer zweidimensionalen Version des PO_4-DOP-Modells basiert, untersuchen wir die Eindeutigkeit numerisch berechneter periodischer Lösungen.

Contents

Introduction

The growing concentration of carbon dioxide (CO_2) in the atmosphere is considered as a main cause of climate change. Understanding and control of climate change therefore requires the understanding of the global carbon cycle. Marine ecosystems are a part of this cycle, and their significance will probably increase because the oceanic carbon uptake is likely to grow corresponding to the higher concentration of CO_2 in the atmosphere. We refer to Stocker et al. [25, Chapters 6, 10] for more details.

Marine ecosystems, more specifically, the biogeochemical processes involved in the oceanic carbon cycle, are described via mathematical models. Well-calibrated models contribute to the understanding of the complex processes and provide a means to simulate the ecosystem's behavior in different scenarios, such as the response to an increased concentration of CO_2. Often, marine ecosystem models include phosphate or nitrogen instead of CO_2. The concentrations of these constituents can be converted into each other by means of the constant Redfield Ratio (cf. Redfield et al. [18]). For information about models, we refer to Fennel and Neumann [6, Section 1.1].

A marine ecosystem model is a system of advection-diffusion-reaction equations. Each equation corresponds to one of the constituents involved in the processes to be described. The constituents can be both of inorganic origin (e.g. carbon, phosphate, iron) and organic origin (e.g. phytoplankton, zooplankton). The solution of one advection-diffusion-reaction equation indicates the concentration of the corresponding constituent depending on space and time. The whole system is referred to as "the model equation", and a solution is a vector of concentrations.

Each concentration is influenced by advection, diffusion, and biogeochemical reactions. Advection is defined as the transport induced by the ocean current. It affects all concentrations equally. For the sake of simplicity, the same is assumed for diffusion. This is a reasonable assumption because turbulent diffusion, which is equal for all constituents, exceeds molecular diffusion notably.

The biogeochemical processes in the ecosystem, such as predator-prey relationships or the growth of phytoplankton depending on insolation, are expressed via reaction (or coupling) terms. Reaction terms can be of varying complexity. Some processes require a nonlinear function depending on space, time, and all modeled concentrations whereas others are described via the product of a concentration with a constant. Sinking processes can be modeled via “nonlocal” reaction terms. These terms include the concentrations at more than one point in space (e.g. an integral over one spatial coordinate).

The reaction terms contain parameters associated with the described processes, such as growth rates, half saturation constants or remineralization rates. Most parameters are constants. However, some situations require temporally and spatially variable parameters (cf. Parekh et al. [15, Sec. 2.3]).

The determination of suitable parameter values is called parameter identification or calibration. Since the model corresponding to such parameter values should reflect reality well, parameter identification can be formulated as an optimization problem. The quantity to be minimized is the difference between observational data and the solution of the model equation, regarded as a function of the parameters. Parameter identification via optimization is an often easier and less expensive alternative to measurements or laboratory experiments.

An important example for a marine ecosystem model is the PO_4-DOP-Fe model by Parekh et al. [15]. It describes the marine phosphorus cycle in relation to the iron cycle by means of the concentrations of phosphate (PO_4), dissolved organic phosphorus (DOP), and iron (Fe). It contains a model of the phosphorus cycle, referred to as PO_4-DOP model or, alternatively, as N-DOP model. The alternative name includes the abbreviation “N” for “nutrient” (cf. Kriest et al. [10, Section 2.2]). Because of its low complexity, the PO_4-DOP model is often used to test numerical methods, for example, in the context of parameter identification (cf. Prieß et al. [17]).

In applications, the model equation and the parameter identification problem are solved numerically. Numerical results are considered adequate if they approximate the solutions of the corresponding continuous problems. Therefore, the validation of numerical results requires an analysis of the continuous problems, especially concerning solvability. For example, if the equation of a continuous model turns out to be unsolvable, the relation between any numerical “solution” and the ecosystem in question will be unknown. Probably, such a model will be dismissed as unreliable. By revealing the reasons for the equation’s deficiency (unsolvability in our example), the analysis can additionally contribute to an improvement of improper models.

Being used for testing purposes, the PO_4-DOP model’s reliability is of particular importance. However, an analysis of the continuous PO_4-DOP model is not available so far. The same is true for all other models that are known to us. Therefore, this work is dedicated to the mathematical analysis of a preferably large class of ecosystem models including the PO_4-DOP model. We explicitly use the attribute “mathematical” to point out that we only consider existing models. The actual modeling of biogeochemical processes, i.e., the finding of the model’s formulation, is not a part of this work.

The mathematical analysis deals with the solvability of the model equation, uniqueness of solutions, and the parameter identification problem.

In the first part, we investigate weak solutions, i.e., solutions of a weak formulation of the model equation as is usually done in the context of advection-diffusion equations and optimization with partial differential equations. We regard the weak formulation as a general operator equation in the sense of Gajewski et al. [7] in order to cover both local and nonlocal reaction terms. The weak formulation requires boundary conditions. Normally, homogeneous Neumann boundary conditions, modeling the fact that no material leaves or enters the system through the boundary (seafloor and surface), are chosen in applications (e.g. in Prieß et al. [17, Section 2.1]). However, these conditions conflict with conservation of mass if material accumulates at the boundary (e.g. after sinking). This is the case in the PO_4-DOP model, for instance. Thus, we admit nonlinearly coupled Neumann boundary conditions in this work.

Different types of weak solutions are distinguished by a condition for the initial value, i.e., the solution's value at the point of time $t = 0$.

Transient solutions on the finite time interval $[0, T]$ are characterized by a prescribed initial value. Transient weak solutions of single partial differential equations or operator equations are well investigated. In literature, different methods are applied according to the properties of the equation's summands. Evans [5, Theorem 9.2] uses Banach's Fixed Point Theorem to solve a nonlinear equation with Lipschitz continuous summands. Galerkin's method is applied to monotone or linear summands by Ladyzhenskaya et al. [11], Tröltzsch [26] and Gajewski et al. [7], for instance, and to pseudo-monotone and coercive operators by Růžička [19]. Casas [2] uses a truncation method for problems with monotone boundary conditions. However, the assumptions of the available existence results practically never apply to all reaction terms of a marine ecosystem model simultaneously. For example, the main reason for missing monotonicity and coercivity is the coupling of the modeled constituents because of which many summands appear twice in the equations with different signs. Moreover, the equations investigated by Casas and Tröltzsch, for instance, do not admit nonlocal reaction terms. Finally, all of the cited results address single equations instead of systems.

Periodic solutions on $[0, T]$ are characterized by identical initial and terminal values, i.e., identical values at $t = 0$ and $t = T$. The name "periodic" indicates that these solutions may be extended to a function on $\mathbb{R}$ with period T (see Gajewski et al. [7, Remark VI.1.8]). Periodic solutions are most important in applications since measurements from ecosystems are usually available as an average over several years. Representing a medium year, these "climatological" data correspond to periodic solutions.

Several authors investigate periodic weak solutions. Gajewski et al. [7] consider equations with monotone and coercive operators. Shioji [24] assumes coercivity and pseudo-monotonicity while Sattayatham et al. [23] regard a combination of uniformly monotone and Hölder continuous operators. For the same reasons as in the transient case, none of these results can be directly applied to ecosystem models. A further problem occurs in the context of mass-conserving models, such as the PO_4-DOP model. All included source terms are trivial which has the effect that the constant zero function is a periodic solution. Therefore, results about nontrivial periodic solutions are required in the context of mass-conserving models. The classical existence theorems do not consider nontrivial solvability.

The second part of the analysis is dedicated to the parameter identification problem. We investigate the existence of optimal parameters in both the transient and the periodic case as well as first and second order optimality conditions. These conditions may be the basis for a numerical method which computes optimal parameters.

As a constrained optimization problem for partial differential equations, parameter identification is an optimal control problem (see e.g. Tröltzsch [26]). Using a standard method, Hinze et al. [9, Section 1.5.2] prove a general existence theorem about optimal parameters which requires the unique solvability of the model equation. Since this property is not fulfilled in the periodic case, the standard theorem is not immediately applicable. The same is true for the standard results about optimality conditions.

This work is structured according to the topics indicated above.

In the first section of Chapter 1, we shortly introduce our notation and recapitulate definitions and theorems that are used in this work. The remaining sections of this chapter are dedicated to the mathematical formulation of a general marine ecosystem model. We provide the classical formulation and shortly repeat the derivation of a weak formulation. The important step is the transition to the corresponding operator equation which is the object of all subsequent investigations. In Section 1.5, we define the important quantity "mass" and prove a characterization of mass-conserving models.

Chapter 2 includes two results about existence and uniqueness of transient weak solutions. Both theorems treat models with reaction terms consisting of monotone and Lipschitz continuous summands. The first theorem is proved by means of Galerkin's method which we adapt to systems of equations and the two types of reaction terms. To prove the second existence theorem, we adapt the method of Evans [5, Section 9.2.1], based on Banach's Fixed Point Theorem, to the ecosystem model equation. The examples at the end of the chapter show one reaction term which is admitted in the regarded model class and one which is not.

Chapter 3 is dedicated to periodic solutions of models of N-DOP type. This model class is introduced in Section 3.1. Like the PO_4-DOP model, models of this class consist of two constituents and reflect remineralization, i.e., the linear transformation of one constituent into another. Furthermore, they are mass-conserving. In the second section, we prove an existence result for nontrivial periodic solutions of models of N-DOP type. The proof relies on the structure of the model equation which enables the application of a standard existence theorem in combination with the Schauder Fixed Point Theorem. The theorem provides different periodic solutions distinguished by mass. This implicates that there are nontrivial solutions (corresponding to a nontrivial mass) and that periodic solutions are not unique. In Section 3.3, we prove the existence of nontrivial stationary solutions. Solving a time-independent version of the model equation, these solutions are of minor importance in applications. We incorporate the existence result nevertheless because it can be proved in the same way as the result about periodic solutions.

In Chapter 4, we deal with the PO_4-DOP model and its extension, the PO_4-DOP-Fe model. In the first three sections, we provide a mathematical formulation of the PO_4-DOP model. We formulate the reaction terms in Section 4.2.2 and derive boundary conditions under the assumption that the model is mass-conserving in Section 4.2.3. In Section 4.3, we determine the mathematical formulation of the reaction terms associated with iron. Section 4.4 contains the application of the existence results, and the last section is dedicated to a numerical method which is typically used to compute periodic solutions. A numerical test based on a two-dimensional version of the PO_4-DOP model sheds light on the question of uniqueness of numerically computed periodic solutions.

The last chapter is concerned with parameter identification. In Section 5.1, we formulate the continuous optimization problem and prove the existence of an optimal parameter for any observational data which are at least quadratically integrable. The existence theorem treats both the transient and the periodic case simultaneously and admits variable parameters. A corollary studies special situations including the case of constant parameters. The section ends with examples of typical reaction terms and parameters to which the existence theorem applies. In Sections 5.2 and 5.3, we give first and second order optimality conditions considering a transient and a periodic model equation, respectively. In addition, we transform the first order condition into an optimality system by adapting the technique of Tröltzsch [26] to parameter identification problems. In the periodic case, the standard technique is not directly applicable since, in general, periodic solutions are not unique. For this reason, we formulate and investigate an alternative optimization problem with a transient model equation instead. In Section 5.4, we investigate the PO_4-DOP model and its parameters with regard to the previously obtained results about parameter identification. In addition, we consider the question, unanswered so far, whether two different parameter values may be associated with the same solution of the PO_4-DOP model. This property is undesired because it affects the reliability of tests. Since some parameters seem to have this property, we suggest an alternative reaction term which is better suited for testing purposes.

Chapter 1

Formulation and properties of the model equation

1.1 Mathematical preliminaries

In the first paragraph, we define the basic objects and abbreviations used in this text. The rest of this section lists important definitions and results from literature.

General assumptions. Throughout this text, let $s, n_p, n_d \in \mathbb{N}$, $n_d \leq 3$ and $T > 0$. Furthermore, let $\Omega \subseteq \mathbb{R}^{n_d}$ be an open, connected and bounded set with a Lipschitz boundary[1] $\Gamma := \partial\Omega$ in case $n_d \geq 2$. The outward-pointing unit normal vector at $s \in \Gamma$ is referred to as $\eta(s)$. We abbreviate $Q_T := \Omega \times (0,T)$ and $\Sigma := \Gamma \times (0,T)$.

Suppose that $\mathbf{v} \in L^\infty(0,T;H^1(\Omega)^{n_d})$ has the properties $\operatorname{div}(\mathbf{v}(t)) = 0$ in Ω and $\mathbf{v}(t)\cdot\eta = 0$ in Γ, each for almost every $t \in [0,T]$. Let $\kappa \in L^\infty(Q_T)$ with $\kappa_{\min} := \operatorname{ess\,inf}\{\kappa(x,t) : (x,t) \in Q_T\} > 0$. Finally, we use the abbreviations $\mathbf{v}_{\max} := \|\mathbf{v}\|_{L^\infty(0,T;H^1(\Omega)^{n_d})}$ and $\kappa_{\max} := \operatorname{ess\,sup}\{\kappa(x,t) : (x,t) \in Q_T\}$.

Norms and spaces. All spaces regarded in this work are implicitly assumed to be real. We use the following notation.

The space of linear and bounded operators between two normed linear spaces B_1 and B_2 will be denoted by $\mathcal{L}(B_1, B_2)$. We use the abbreviation $B_1^* := \mathcal{L}(B_1, \mathbb{R})$ for the continuous dual space of B_1.

The identity map on a normed linear space B is denoted by Id_B.

The Lebesgue measure of a measurable set $M \subseteq \mathbb{R}^{n_d}$ is expressed by $|M|$ instead of $\lambda(M)$.

Norms will usually be distinguished by an index indicating the corresponding space. An exception is made for the Hilbert space $L^2(E)^s$ of s-dimensional vectors of quadratically integrable functions on a set Ψ. Here, we write $\|.\|_{\Psi^s}$ instead of $\|.\|_{L^2(\Psi)^s}$. In the special case $s = 1$, the exponent s is omitted. The same rule applies for inner products in Hilbert

[1] For a definition see e.g. Tröltzsch [26, Section 2.2].

spaces which are defined by round brackets $(.\,,.)$ with the corresponding index. The scalar product in $\mathbb{R}^{n_d}$ is indicated by a dot. The application of a linear functional is denoted by angle brackets $\langle .\,,. \rangle$ subscripted by the corresponding dual space. Dual pairings without any index belong to the space $(H^1(\Omega)^*)^s$.

Furthermore, we use the following definitions and results. Given a Hilbert space H, the Cartesian product H^s is a Hilbert space with the inner product

$$(x, y)_{H^s} := \sum_{i=1}^{s} (x_i, y_i)_H \quad \text{for all } x, y \in H^s.$$

The product Hilbert space is always endowed with the norm induced by this inner product.

Provided that B is a Banach space, the Cartesian product B^s is also a Banach space, endowed with the norm

$$\|x\|_{B^s} := \left(\sum_{i=1}^{s} \|x_i\|_B^2 \right)^{\frac{1}{2}} \quad \text{for all } x \in B^s.$$

The dual space $(B^s)^*$ is isomorphic to $(B^*)^s$. The application of a functional is given by

$$\langle f, v \rangle := \sum_{i=1}^{s} \langle f_i, v_i \rangle_{B^*} \quad \text{for all } f \in (B^*)^s \text{ and } v \in B^s.$$

Let B_1 and B_2 be Banach spaces. The intersection $B := B_1 \cap B_2$, endowed with the norm $\|y\|_B := \|y\|_{B_1} + \|y\|_{B_2}$ for all $y \in B$, is a Banach space as well.

The space B_1 is *continuously embedded* in B_2 (in short: $B_1 \hookrightarrow B_2$) if $B_1 \subseteq B_2$ and the embedding $E_{B_1,B_2} : B_1 \to B_2$, $x \mapsto x$ is continuous. This is equivalent to the existence of a constant $C_{B_1,B_2} > 0$ with $\|x\|_{B_2} \leq C_{B_1,B_2} \|x\|_{B_1}$ for all $x \in B_1$. The space B_1 is *compactly embedded* in B_2 if E_{B_1,B_2} is a compact operator.

The following theorem provides a means to "restrict" elements of $H^1(\Omega)$ to the boundary of Ω. The proof can be found in Evans [5, Section 5.5].

Theorem 1.1.1. (Trace Theorem) *There is a linear and continuous map $\tau : H^1(\Omega) \to L^2(\Gamma)$ that restricts continuous functions $y \in H^1(\Omega) \cap C(\bar{\Omega})$ to the boundary, i.e., $(\tau y)(x) = y(x)$ for all $x \in \Gamma$. The continuity of τ implies the existence of a constant $c_\tau > 0$, depending solely on Ω, with the property $\|\tau y\|_{L^2(\Gamma)} \leq c_\tau \|y\|_{H^1(\Omega)}$ for all $y \in H^1(\Omega)$.*

Evolution triples. Proofs and further information about the following definitions can be found in Zeidler [30, Chapter 23] or Gajewski et al. [7].

An *evolution triple* (V, H, V^*) consists of a real and separable Hilbert space H and a real, reflexive and separable Banach space V that is continuously embedded and lies dense in H. Because of the theorem of Fréchet-Riesz, every element of H can be identified with an element of H^*. Furthermore, H^* is embedded in V^*. Shortly, these relations are indicated by the notation $V \subseteq H \subseteq V^*$. Given the evolution triple (V, H, V^*), we define the space

$$W(0,T;V) := \{y \in L^2(0,T;V) : \, y' \in L^2(0,T;V^*)\}.$$

The space $L^2(0,T;V^*)$ can be identified with the dual space of $L^2(0,T;V)$ (Gajewski et al. [7, Theorem IV.1.14]). We will write $L^2(0,T;V^*)$ instead of $L^2(0,T;V)^*$ throughout this text. For a formal definition of the weak derivative y', we refer to Zeidler [30].

The following theorem gathers some important facts about an evolution triple (V, H, V^*).

Theorem 1.1.2. *The following properties are valid:*

1. *The space $W(0,T;V)$ is continuously embedded in $C([0,T];H)$, i.e., there exists a constant $C_E > 0$ with*

$$\|y\|_{C([0,T];H)} \leq C_E \|y\|_{W(0,T;V)} \quad \text{for all } y \in W(0,T;V).$$

2. *For all $y \in W(0,T;V)$, the map $t \mapsto \|y(t)\|_H^2$ is differentiable almost everywhere with $\frac{d}{dt}\|y(t)\|_H^2 = 2\langle y'(t), y(t)\rangle_{V^*}$.*
3. *Let $y, v \in W(0,T;V)$. Then, the formula of integration by parts*

$$\int_0^T \langle y'(t), v(t)\rangle_{V^*} dt + \int_0^T \langle v'(t), y(t)\rangle_{V^*} dt = (y(T), v(T))_H - (y(0), v(0))_H$$

holds. In particular, this implies the "fundamental theorem"

$$\int_0^T \langle y'(t), y(t)\rangle_{V^*} dt = \frac{1}{2}\left(\|y(T)\|_H^2 - \|y(0)\|_H^2\right).$$

The first statement implies that an element of $W(0,T;V)$ can be evaluated at every $t \in [0,T]$. In connection with the frequently used evolution triple $(H^1(\Omega), L^2(\Omega), H^1(\Omega)^*)$, we use the abbreviation $W(0,T) := W(0,T;H^1(\Omega))$.

Operators. Let (V, H, V^*) be an evolution triple and Y be a Banach space in which $W(0,T;V)$ is continuously embedded. We abbreviate $X := L^2(0,T;V)$. The operator $A : Y \to X^*$ is *generated by the indexed family* $(A(t))_t$ if there exist a space $\Lambda \subseteq H$ with the property

$$y(t) \in \Lambda \text{ for all } y \in Y \text{ and almost all } t \tag{1.1}$$

and operators $A(t) : \Lambda \to V^*$ with $A(t)(y(t)) = [A(y)](t)$ or, in other words,

$$\langle A(y), v\rangle_{L^2(0,T;V^*)} = \int_0^T \langle A(t)(y(t)), v(t)\rangle_{V^*} dt \quad \text{for all } y \in Y, v \in X \tag{1.2}$$

(cf. Gajewski [7, Remark VI.1.2]). If there is no danger of confusion, we write $A(y(t))$ instead of $A(t)(y(t))$.

Let additionally $Y \hookrightarrow X$ be valid. The operator A is called

- *monotone* if $\langle Ay - Av, y - v\rangle_{X^*} \geq 0$ for all $y, v \in Y$,
- *strictly monotone* if $\langle Ay - Av, y - v\rangle_{X^*} > 0$ for all $y, v \in Y$ with $y \neq v$,
- *coercive* if $\|y\|_Y \to \infty$ implies $\langle Ay, y\rangle_{X^*}/\|y\|_Y \to \infty$,
- *hemicontinuous* if the map $t \mapsto \langle A(y + tv), w\rangle_{X^*}$ is continuous at every $t \in [0, 1]$ for all $y, v, w \in Y$,
- *demicontinuous* if the image of a strongly convergent sequence in Y is weakly convergent in X^*,
- *weakly (sequentially) continuous* if the image of a weakly convergent sequence in Y is weakly convergent in X^*,
- *strongly continuous* if the image of a weakly convergent sequence in Y is strongly convergent in X^*.

The following theorem is concerned with periodic solutions of operator equations.

Theorem 1.1.3 (Existence theorem of Gajewski et al. [7])**.** *If $A : X \to X^*$ is a hemicontinuous, monotone, and coercive operator, the problem*

$$y' + Ay = f, \quad y(0) = y(T),$$

has a solution $y \in W(0, T; V)$ for every $f \in X^*$. If A is strictly monotone, the solution is unique.

1.2 Equations in classical form

The following hypothesis introduces the reaction and source terms of a general ecosystem model.

Hypothesis 1.2.1. *Let Y be a Banach space. Suppose that $W(0, T)^s$ is continuously embedded in Y and that $\Lambda \subseteq L^2(\Omega)^s$ fulfills the property* (1.1)*. For every $i \in \{1, \ldots, n_p\}$, let U_i be a Banach space of functions on Q_T or Σ and $U := U_1 \times \ldots \times U_{n_p}$. Furthermore, let $V \subseteq U$. We assume that the reaction terms*

$$d : V \times Y \to L^2(Q_T)^s \text{ and } b : V \times Y \to L^2(\Sigma)^s$$

fulfill the following property: For every fixed $u \in V$, there are indexed families $(d(t))_t$ and $(b(t))_t$ of operators

$$d(t) : \Lambda \to L^2(\Omega)^s \text{ and } b(t) : \Lambda \to L^2(\Gamma)^s$$

satisfying $d(u, y)(x, t) = d(t)(y(t))(x)$ *for all* $y \in Y$ *and almost all* $(x, t) \in Q_T$ *and an analogous identity for* b.

Let furthermore $q_{Q_T} : V \to L^2(Q_T)^s$ *and* $q_\Sigma : V \to L^2(\Sigma)^s$ *be the source terms.*

Provided that Hypothesis 1.2.1 holds, a marine ecosystem model is given by the s-dimensional system of advection-diffusion-reaction equations with boundary conditions

$$\begin{aligned} \partial_t y_j + \mathbf{v} \cdot \nabla y_j - \operatorname{div}(\kappa \nabla y_j) + d_j(u, y) &= q_{Q_T j}(u) \quad \text{in } Q_T \\ \nabla y_j \cdot (\kappa \eta) + b_j(u, y) &= q_{\Sigma j}(u) \quad \text{in } \Sigma \end{aligned} \tag{1.3}$$

for all $j \in \{1, \ldots, s\}$. The system (1.3) and the associated operator equation (cf. Equation (1.6) below) are both referred to as "the model equation".

In all chapters except for Chapter 5 about parameter identification, we regard the model with a fixed parameter u. For this reasons, we omit the argument u of d, b, q_{Q_T}, and q_Σ. In Chapter 5, we will return to the original notation introduced in Hypothesis 1.2.1.

1.3 Weak formulation

Let Hypothesis 1.2.1 be valid. Weak solutions of the system (1.3) have less regularity than classical solutions in $C^2(\bar{Q}_T)^s$. However, it is required that weak and classical solutions coincide as soon as the latter exist. Therefore, the following derivation of a weak formulation takes a classical solution of the s-dimensional system (1.3) as a starting point.

Suppose that $y \in C^2(\bar{Q}_T)^s \subseteq Y$ is a solution of (1.3) and let $w \in C^1(\bar{Q}_T)^s$ be a vector of test functions. In the first step, the j-th model equation, evaluated at $(x, t) \in \Omega \times [0, T]$, is multiplied by $w_j(x, t)$. Integrating with respect to Ω, we obtain

$$\begin{aligned} (\partial_t y_j(t), w_j(t))_\Omega + (\mathbf{v}(t) \cdot \nabla y_j(t), w_j(t))_\Omega - (\operatorname{div}(\kappa(t) \nabla y_j(t)), w_j(t))_\Omega + (d_j(y, .\,, t), w_j(t))_\Omega \\ = (q_{Q_T j}(t), w_j(t))_\Omega \end{aligned}$$

for every $j \in \{1, \ldots, s\}$. To relax the regularity of y_j, we interpret the temporal derivative $\partial_t y_j$ as a distributional derivative, i.e.,

$$(\partial_t y_j(t), w_j(t))_\Omega = \langle y_j'(t), w_j(t) \rangle_{H^1(\Omega)^*}.$$

The third summand is transformed using integration by parts based on Gauß' divergence theorem. Inserting the boundary condition, we obtain

$$\begin{aligned} -\int_\Omega \operatorname{div}(\kappa \nabla y_j) w_j dx &= \int_\Omega (\kappa \nabla y_j \cdot \nabla w_j) dx - \int_\Gamma (\nabla y_j \cdot (\kappa \eta)) w_j d\sigma \\ &= \int_\Omega (\kappa \nabla y_j \cdot \nabla w_j) dx + \int_\Gamma (b_j(y, \sigma, t) - q_{\Sigma j}) \, w_j d\sigma. \end{aligned}$$

In the majority of cases, we omitted the arguments (x, t) and (σ, t).

All linear summands are gathered in the time-dependent bilinear form $B^s : H^1(\Omega)^s \times H^1(\Omega)^s \times [0,T] \to \mathbb{R}$, given by $B^s(z,v;t) := \sum_{j=1}^{s} B(z_j, v_j; t)$ with B defined by

$$B(z_j, v_j; t) := \int_\Omega (\kappa(t)\nabla z_j \cdot \nabla v_j)dx + \int_\Omega (\mathbf{v}(t) \cdot \nabla z_j)v_j dx.$$

The first statement of Lemma 1.4.2 below ensures that B and B^s are well-defined. Later, we apply B^s mostly to the values of abstract functions $\alpha, \beta \in L^2(0,T;H^1(\Omega))^s$ at a fixed t. In this case, we write $B^s(\alpha, \beta; t)$ instead of $B^s(\alpha(t), \beta(t); t)$.

The previous steps lead to the weak formulation

$$\begin{aligned}\langle y_j'(t), w_j(t)\rangle_{H^1(\Omega)^*} + B(y_j, w_j; t) + (d_j(y, .\,, t), w_j(t))_\Omega + (b_j(y, .\,, t), w_j(t))_\Gamma \\ = (q_{Q_T j}(t), w_j(t))_\Omega + (q_{\Sigma j}(t), w_j(t))_\Gamma\end{aligned}$$

for all $t \in [0,T]$ and all test functions. We obtain a weak formulation for the s-dimensional problem by integrating with respect to time and summing up the equations for all $j \in \{1, \ldots, s\}$. Because of Lemma 1.4.1 in the next section, the summands associated with reaction and source terms are well-defined for all $y \in Y$ and $w \in L^2(0,T;H^1(\Omega))^s$. Moreover, the first summand requires $y' \in L^2(0,T;H^1(\Omega)^*)^s$, and B^s admits arguments belonging to $L^2(0,T;H^1(\Omega))^s$. Thus, $W(0,T)^s$ is an adequate solution space.

According to these considerations, a weak solution $y \in W(0,T)^s$ fulfills

$$\begin{aligned}\int_0^T \{\langle y'(t), w(t)\rangle + B^s(y, w; t) + (d(y, .\,, t), w(t))_{\Omega^s} + (b(y, .\,, t), w(t))_{\Gamma^s}\}dt \\ = \int_0^T \{(q_{Q_T}(t), w(t))_{\Omega^s} + (q_\Sigma(t), w(t))_{\Gamma^s}\}dt \qquad (1.4)\end{aligned}$$

for all test functions $w \in L^2(0,T;H^1(\Omega))^s$.

1.4 Weak formulation as operator equation

Many results about weak solutions are obtained using the theory of operator equations. To adapt our problem to this framework, we prove that the summands of the weak formulation (1.4) can be identified with operators mapping into $L^2(0,T;H^1(\Omega)^*)^s$.

First, we address the reaction and source terms (cf. Tröltzsch [26, Theorem 3.12]).

Lemma 1.4.1. *Let Hypothesis 1.2.1 be valid. For every $y \in Y$, the definition*

$$F(y) : w \mapsto \int_0^T [(d(y, .\,, t), w(t))_{\Omega^s} + (b(y, .\,, t), \tau w(t))_{\Gamma^s}]dt \quad \textit{for all } w \in L^2(0,T;H^1(\Omega))^s$$

describes the operator $F : Y \to L^2(0,T;H^1(\Omega)^*)^s$ which is generated by the indexed family

$(F(t))_t$ of operators $F(t) : \Lambda \to (H^1(\Omega)^*)^s$ with

$$F(t)(v) : z \mapsto (d(t)(v), z)_{\Omega^s} + (b(t)(v), \tau z)_{\Gamma^s} \qquad \text{for all } v \in \Lambda, z \in H^1(\Omega)^s$$

in the sense of (1.2)*. Moreover, the map f, defined by*

$$\langle f, w\rangle_{L^2(0,T;H^1(\Omega)^*)^s} := \int_0^T \{(q_{Q_T}(t), w(t))_{\Omega^s} + (q_\Sigma(t), \tau w(t))_{\Gamma^s}\} dt$$

for all $w \in L^2(0,T;H^1(\Omega))^s$, is an element of $L^2(0,T;H^1(\Omega)^*)^s$.

In the formulation of the lemma, we use the trace operator τ of Theorem 1.1.1 to point out the different domains of integration in both integrals. Later, we will return to omitting τ in the boundary integrals.

Proof. The operator F is generated by $(F(t))_t$ in the sense of (1.2) because of the relationship between d, b and $(d(t))_t, (b(t))_t$ given in Hypothesis 1.2.1. Thus, it remains to be shown that all operators specified in the lemma are well-defined. We start with the indexed family. Let $v \in \Lambda$ and $z \in H^1(\Omega)^s$. The operator $F(t)(v)$ belongs to $(H^1(\Omega)^*)^s$ if it is linear and bounded. The first property holds by definition. Regarding the second, we conclude with the Cauchy-Schwarz inequality in $L^2(\Gamma)^s$ and Theorem 1.1.1

$$(b(t)(v), \tau z)_{\Gamma^s} \leq \|b(t)(v)\|_{\Gamma^s}\|\tau z\|_{\Gamma^s} \leq \|b(t)(v)\|_{\Gamma^s} c_\tau \|z\|_{H^1(\Omega)^s}.$$

Similarly, we obtain $(d(t)(v), z)_{\Omega^s} \leq \|d(t)(v)\|_{\Omega^s}\|z\|_{H^1(\Omega)^s}$. Thus,

$$\|F(t)(v)\|_{(H^1(\Omega)^*)^s} \leq \|d(t)(v)\|_{\Omega^s} + \|b(t)(v)\|_{\Gamma^s} c_\tau.$$

The upper bound is finite because $d(t)(v) \in L^2(\Omega)^s$ and $b(t)(v) \in L^2(\Gamma)^s$.

We proceed with the operator involving time. Given $y \in Y$, the norm of $F(y)$ is equal to the integral over the norm of $F(y(t))$ because of (1.2). Using the estimate of the generating functional and the convexity of the square function on $\mathbb{R}$, we obtain

$$\|F(y)\|^2_{L^2(0,T;H^1(\Omega)^*)^s} = \int_0^T \|F(y(t))\|^2_{(H^1(\Omega)^*)^s} dt \leq 2\left(\|d(y)\|^2_{L^2(Q_T)^s} + \|b(y)\|^2_{L^2(\Sigma)^s} c_\tau^2\right). \quad (1.5)$$

The last expression is finite due to the assumptions about d and b.

The statement about f can be proved by means of the same arguments because f and $F(y)$ are defined in an analogous way. □

The bilinear form $B^s(.,.)$ can be identified with the linear operator

$$B^s : L^2(0,T;H^1(\Omega))^s \to L^2(0,T;H^1(\Omega)^*)^s, \ \langle B^s(z), v\rangle_{L^2(0,T;H^1(\Omega)^*)} := \int_0^T \sum_{j=1}^s B(z_j, v_j; t) dt$$

for all $z, v \in L^2(0,T;H^1(\Omega))^s$, generated by the family $(B^s(t))_t$ consisting of $B^s(t) : H^1(\Omega)^s \to (H^1(\Omega)^*)^s$ with $B^s(t)(w) := B^s(w, .\,; t)$ for all $w \in H^1(\Omega)^s$. The first statement of Lemma 1.4.2 below in combination with Hölder's inequality in $L^2(0,T)$ ensures that the operators B^s and $B^s(t)$ are well-defined.

Using the previous definitions, we can formulate the weak formulation as the operator equation

$$y' + B^s(y) + F(y) = f \quad \text{in } L^2(0,T;H^1(\Omega)^*)^s. \tag{1.6}$$

A solution y of this equation belongs to $W(0,T)^s$.

We conclude this section with some important statements concerning the bilinear form $B^s(\,.\,,.\,;t)$ and the operator B^s.

Lemma 1.4.2. *Let $1 \in H^1(\Omega)$ be the constant function that is equal to one almost everywhere. The following properties hold for all $y, v \in H^1(\Omega)^s$ and almost all $t \in [0,T]$.*

1. *There is a constant $C_B > 0$, independent of t, y, v, such that*

$$|B^s(y,v;t)| \leq C_B \|y\|_{H^1(\Omega)^s} \|v\|_{H^1(\Omega)^s}.$$

2. $\kappa_{\min}\|y\|^2_{H^1(\Omega)^s} \leq B^s(y,y;t) + \kappa_{\min}\|y\|^2_{L^2(\Omega)^s}$. *In particular,* $B^s(y,y;t) \geq 0$.
3. $B(y_j, 1; t) = 0$ *for all* $j \in \{1, \dots, s\}$.
4. $B(y_j + c, v_j; t) = B(y_j, v_j; t)$ *for every measurable function* $c : [0,T] \to \mathbb{R}$ *and all* $j \in \{1, \dots, s\}$.
5. *The operator B^s is monotone.*

The proof of Lemma 1.4.2 uses the following auxiliary lemma.

Lemma 1.4.3. *Let $v \in H^1(\Omega)^{n_d}$ with $\mathrm{div} v = 0$ in Ω and $v \cdot \eta = 0$ in Γ. Hence,*

$$\int_\Omega (v \cdot \nabla w) w dx = 0 \quad \textit{for all } w \in H^1(\Omega).$$

Proof. Let $w \in H^1(\Omega)$. For all $c \in H^1(\Omega)$ und $x \in H^1(\Omega)^{n_d}$, we obtain

$$\mathrm{div}(cx) = \sum_{i=1}^{n_d} \partial_i(cx_i) = \sum_{i=1}^{n_d} (c(\partial_i x_i) + x_i(\partial_i c)) = c \sum_{i=1}^{n_d} \partial_i x_i + \sum_{i=1}^{n_d} x_i(\partial_i c) = c\,\mathrm{div} x + x \cdot \nabla c,$$

a product rule for the divergence. This formula applied to $c := w$ and $x := v$ yields

$$\int_\Omega \mathrm{div}(vw) w dx = \int_\Omega w^2 \mathrm{div} v dx + \int_\Omega (v \cdot \nabla w) w dx = \int_\Omega (v \cdot \nabla w) w dx.$$

The summand with w^2 vanishes because of the assumption about the divergence of v. By means of the product rule applied to $c := w$ and $x := vw$, the same integral proves equal to an integral over the divergence of vw^2 which can be transformed into a boundary integral by virtue of Gauß' divergence theorem. In detail, we obtain

$$\begin{aligned}\int_\Omega \operatorname{div}(vw)w dx &= \int_\Omega \operatorname{div}(vw^2)dx - \int_\Omega ((vw)\cdot\nabla w)dx \\ &= \int_\Gamma (v\cdot\eta)w^2 d\sigma - \int_\Omega (v\cdot\nabla w)w dx = -\int_\Omega (v\cdot\nabla w)w dx.\end{aligned}$$

The first integral in the second line vanishes because the product of v with the outward-pointing normal η is assumed to be zero. The difference of the last two equations is equal to

$$2\int_\Omega (v\cdot\nabla w)w dx = \int_\Omega \operatorname{div}(vw)w dx - \int_\Omega \operatorname{div}(vw)w dx = 0.$$

This equality implies the statement of the lemma. □

Proof of Lemma 1.4.2. Throughout this proof, let $y, v \in H^1(\Omega)^s$, $j \in \{1,\dots,s\}$, and $t \in [0,T]\setminus M$ with M being a suitable subset of $[0,T]$ with $|M| = 0$.

We start proving the first statement for the summand $B(y_j, v_j; t)$. The Cauchy-Schwarz inequality in $L^2(\Omega)^{n_d}$ yields

$$\left|\int_\Omega (\kappa(t)\nabla y_j\cdot\nabla v_j)dx\right| \le \kappa_{\max}\,|(\nabla y_j,\nabla v_j)_{\Omega^{n_d}}| \le \kappa_{\max}\|\nabla y_j\|_{\Omega^{n_d}}\|\nabla v_j\|_{\Omega^{n_d}} \quad \text{and}$$

$$\left|\int_\Omega (\mathbf{v}(t)\cdot\nabla y_j)v_j dx\right| = |(\mathbf{v}(t)v_j,\nabla y_j)_{\Omega^{n_d}}| \le \|\mathbf{v}(t)v_j\|_{\Omega^{n_d}}\|\nabla y_j\|_{\Omega^{n_d}}.$$

For every $i \in \{1,\dots,n_d\}$, Hölder's inequality with the exponents $p = \frac{3}{2}$ and $q = 3$ provides

$$\|\mathbf{v}_i(t)v_j\|_\Omega = \left(\int_\Omega \mathbf{v}_i(t)^2 v_j^2 dx\right)^{\frac{1}{2}} \le \left(\int_\Omega \mathbf{v}_i(t)^3 dx\right)^{\frac{1}{3}}\left(\int_\Omega v_j^6 dx\right)^{\frac{1}{6}} = \|\mathbf{v}_i(t)\|_{L^3(\Omega)}\|v_j\|_{L^6(\Omega)}$$

and therefore

$$\|\mathbf{v}(t)v_j\|_{\Omega^{n_d}} = \left(\sum_{i=1}^{n_d}\|\mathbf{v}_i(t)v_j\|_\Omega^2\right)^{\frac{1}{2}} \le \left(\sum_{i=1}^{n_d}\|\mathbf{v}_i(t)\|_{L^3(\Omega)}^2\|v_j\|_{L^6(\Omega)}^2\right)^{\frac{1}{2}} = \|\mathbf{v}(t)\|_{L^3(\Omega)^{n_d}}\|v_j\|_{L^6(\Omega)}.$$

For each $r \in \{3,6\}$, $H^1(\Omega)$ is continuously embedded in $L^r(\Omega)$. Thus, there is a constant $c_r > 0$ with $\|w\|_{L^r(\Omega)} \le c_r\|w\|_{H^1(\Omega)}$ for all $w \in H^1(\Omega)$. We estimate

$$\left|\int_\Omega (\mathbf{v}(t)\cdot\nabla y_j)v_j dx\right| \le c_3\|\mathbf{v}(t)\|_{H^1(\Omega)^{n_d}}c_6\|v_j\|_{H^1(\Omega)}\|\nabla y_j\|_{\Omega^{n_d}} \le \mathbf{v}_{\max}c_3c_6\|v_j\|_{H^1(\Omega)}\|y_j\|_{H^1(\Omega)}.$$

Combining the results, we obtain

$$|B(y_j, v_j; t)| \leq C_B \|y_j\|_{H^1(\Omega)} \|v_j\|_{H^1(\Omega)}$$

with the constant $C_B := \kappa_{\max} + \mathbf{v}_{\max} c_3 c_6$. The Cauchy-Schwarz inequality in $\mathbb{R}^s$ yields the assertion for B^s.

To prove the second statement for $B(y_j, y_j; t)$, we observe primarily that the summand containing $\mathbf{v}$ vanishes according to Lemma 1.4.3, applied to $\mathbf{v}(t)$ and y_j. We estimate the summand containing diffusion by

$$\int_\Omega \kappa(t)(\nabla y_j \cdot \nabla y_j) dx \geq \kappa_{\min} \int_\Omega (\nabla y_j \cdot \nabla y_j) dx = \kappa_{\min} \|\nabla y_j\|^2_{\Omega^{n_d}}.$$

Hence,

$$\kappa_{\min} \|\nabla y_j\|^2_{\Omega^{n_d}} \leq B(y_j, y_j; t). \tag{1.7}$$

Finally, we add $\kappa_{\min}\|y_j\|^2_\Omega$ on both sides of (1.7). The sum of the resulting inequalities for $j \in \{1, \dots, s\}$ corresponds to the assertion. The sum of (1.7) for $j \in \{1, \dots, s\}$ yields the additional assertion of (2).

Before proving the third statement, we observe that the product rule for the divergence in the proof of Lemma 1.4.3, applied to $c := y_j$ and $x := \mathbf{v}(t)$, in combination with the assumption about $\mathbf{v}(t)$ yields $\operatorname{div}(\mathbf{v}(t)y_j) = y_j \operatorname{div}(\mathbf{v}(t)) + \mathbf{v}(t) \cdot \nabla y_j = \mathbf{v}(t) \cdot \nabla y_j$. This equality admits the transformation of the second summand of $B(y_j, 1; t)$. In addition, we apply Gauß' divergence theorem and the assumption about $\mathbf{v}$. We obtain

$$B(y_j, 1; t) = \int_\Omega (\kappa \nabla y_j \cdot \nabla 1) dx + \int_\Omega \operatorname{div}(\mathbf{v}(t) y_j) 1 dx = 0 + \int_\Gamma (\mathbf{v}(t) y_j) \cdot \eta d\sigma = \int_\Gamma y_j (\mathbf{v}(t) \cdot \eta) d\sigma = 0.$$

To prove the fourth assertion, we regard $c(t)$ as an element of $H^1(\Omega)$ which is independent of x. We obtain

$$B(c(t), v_j; t) = c(t) \left(\int_\Omega (\kappa(t) \nabla 1 \cdot \nabla v_j(t)) dx + \int_\Omega (\mathbf{v}(t) \cdot \nabla 1) v_j(t) dx \right) = 0.$$

The original assertion holds because B is bilinear.

Let $w, z \in L^2(0, T; H^1(\Omega))^s$. The last assertion is a consequence of the additional statement of (2) applied to $w(t) - z(t)$ instead of y. Additionally considering the definition of the operator B^s and the bilinearity of $B^s(\,.\,,.\,;t)$, we conclude

$$\langle B^s(w) - B^s(z), w - z \rangle_{L^2(0,T;H^1(\Omega)^*)} = \int_0^T B^s(w - z, w - z; t) dt \geq 0.$$

Thus, the lemma is proved. □

1.5 Conservation of mass

Many ecosystem models are designed to describe cycles, such as the phosphorus cycle. In this case, the model equation usually lacks external sources and sinks, i.e., $q_{Q_T} = 0$ and $q_\Sigma = 0$ as well as $d(0) = 0$ and $b(0) = 0$. Moreover, no material leaves or enters the system through the boundary (seafloor and surface). These conditions imply that the total mass in the ecosystem remains constant with respect to time. Conservation of mass is a crucial property when it comes to the analysis of periodic solvability.

In this section, we formalize the concept of mass and indicate a condition under which the reaction and source terms ensure that an ecosystem model is mass-conserving.

The mass can be defined very generally.

Definition 1.5.1.

- *The function*

$$\text{mass} : L^1(\Omega)^s \to \mathbb{R}, \quad \text{mass}(v) := \sum_{j=1}^{s} \int_\Omega v_j dx$$

relates any vector of functions on Ω to its total mass in Ω.

- *An s-dimensional vector of concentrations $y \in C([0,T]; L^1(\Omega))^s$ has a constant mass if there exists $C \in \mathbb{R}$ with*

$$\text{mass}(y(t)) = C \quad \textit{for all } t \in [0,T].$$

The mass of a solution $y \in W(0,T)^s$ of an ecosystem model will prove weakly differentiable with respect to time. In this case, "having a constant mass" can be characterized by a vanishing derivative.

Proposition 1.5.2. *Let $y \in C([0,T]; L^1(\Omega))^s$ such that*

$$\text{mass}(y) : [0,T] \to \mathbb{R},\ t \mapsto \text{mass}(y(t))$$

is an element of $H^1(0,T)$. Then, y has a constant mass if and only if $\frac{d}{dt}\text{mass}(y) = 0$.

Proof. The first implication holds because the (weak) derivative of every constant function is zero.

Regarding the second implication, mass(y) is constant almost everywhere because the weak derivative with respect to time vanishes. In addition, the choice of y implies that mass(y) is continuous. Thus, there exists $C \in \mathbb{R}$ with $\text{mass}(y(t)) = C$ for all $t \in [0,T]$. □

By means of this characterization, we are able to prove a sufficient property of models conserving mass.

Theorem 1.5.3. *Let Y be a Banach space with $W(0,T)^s \hookrightarrow Y$. Consider the functional $\tilde{f} \in L^2(0,T; H^1(\Omega)^*)^s$ and the operator $\tilde{F} : Y \to L^2(0,T; H^1(\Omega)^*)^s$, generated by the family* *of operators* $\tilde{F}(t) : \Lambda \to (H^1(\Omega)^*)^s$ *with* $\Lambda \subseteq L^2(\Omega)^s$ *fulfilling property* (1.1). *By 1 we denote the element of* $H^1(\Omega)$ *that is equal to one almost everywhere. Suppose that the operator equation*

$$y' + B^s(y) + \tilde{F}(y) = \tilde{f}$$

has a solution $y \in W(0,T)^s$. *If the "conservation of mass conditions"*

$$\sum_{j=1}^{s} \langle \tilde{F}_j(z(t)), 1\rangle_{H^1(\Omega)^*} = 0 \quad \textit{and} \quad \sum_{j=1}^{s} \langle \tilde{f}_j(t), 1\rangle_{H^1(\Omega)^*} = 0 \tag{1.8}$$

are fulfilled for almost all $t \in [0,T]$ *and all* $z \in Y$, *the function* mass(y) *defined in Proposition 1.5.2 is weakly differentiable and the weak derivative is equal to zero almost everywhere. In particular, the solution* y *has a constant mass.*

Lemma 1.4.1 immediately yields the following remark, stating that reaction and source terms of mass-conserving models cancel each other out in some sense.

Remark 1.5.4. *If the operator equation of Theorem 1.5.3 corresponds to the weak formulation of an ecosystem model, the operator* $\tilde{F}$ *and the right-hand side* $\tilde{f}$ *are defined by reaction and source terms according to Lemma 1.4.1. In this case, the conservation of mass conditions* (1.8) *are equal to*

$$\sum_{j=1}^{s} \left(\int_\Omega d_j(z,x,t)dx + \int_\Gamma b_j(z,\sigma,t)d\sigma \right) = 0$$

and

$$\sum_{j=1}^{s} \left(\int_\Omega q_{Q_T j}(x,t)dx + \int_\Gamma q_{\Sigma j}(\sigma,t)d\sigma \right) = 0$$

for all $z \in Y$ *and almost every* $t \in [0,T]$.

Proof of Theorem 1.5.3. Let the conservation of mass conditions (1.8) be valid, and let $y \in W(0,T)^s$ be a solution of the operator equation specified in the theorem.

To show that mass(y) is weakly differentiable, let $\varphi \in C_0^\infty(0,T)$ be a test function. Since the support of φ is compact in $(0,T)$, we have $\varphi(0) = \varphi(T) = 0$. The test function φ can be interpreted as an element of $W(0,T)$ that is constant with respect to x. In this case, we identify the derivative φ' with the element of $L^2(0,T;H^1(\Omega)^*)$ given by

$$\int_0^T \langle \varphi'(t), v(t)\rangle_{H^1(\Omega)^*} dt = \int_0^T \varphi'(t) \int_\Omega v(t)dxdt \quad \text{for all } v \in L^2(0,T;H^1(\Omega)).$$

The definition of mass$(y(t))$, the equation for φ', and Theorem 1.1.2(3) yield

$$-\int_0^T \text{mass}(y(t))\varphi'(t)dt = -\int_0^T \varphi'(t) \int_\Omega \sum_{j=1}^{s} y_j(t)dxdt = -\int_0^T \langle \varphi'(t), \sum_{j=1}^{s} y_j(t)\rangle_{H^1(\Omega)^*} dt$$

$$= \sum_{j=1}^{s} \left(\int_0^T \langle y_j'(t), \varphi(t) \rangle_{H^1(\Omega)^*} dt - (\varphi(T), y_j(T))_{L^2(\Omega)} + (\varphi(0), y_j(0))_{L^2(\Omega)} \right).$$

The summands with $\varphi(0)$ and $\varphi(T)$ vanish since $\varphi \in C_0^\infty(0,T)$. The operator equation at $(\varphi, \dots, \varphi) \in L^2(0,T; H^1(\Omega))^s$ yields for the first summand

$$\sum_{j=1}^{s} \int_0^T \langle y_j'(t), \varphi(t) \rangle_{H^1(\Omega)^*} dt$$
$$= \sum_{j=1}^{s} \int_0^T \left(\langle \tilde{f}_j(t), 1 \rangle_{H^1(\Omega)^*} - B(y_j, 1; t) - \langle \tilde{F}_j(y(t)), 1 \rangle_{H^1(\Omega)^*} \right) \varphi(t) dt = 0.$$

The right-hand side is equal to zero because of Lemma 1.4.2(3), the assumed conditions (1.8), and $y \in Y$. Hence, mass(y) is weakly differentiable, and the weak derivative is equal to zero almost everywhere. Since $y \in W(0,T)^s$ can be identified with an element of $C([0,T]; L^2(\Omega))^s$ according to Theorem 1.1.2(1), the additional assertion of the theorem follows from Proposition 1.5.2. □

1.6 Types of solution

We are basically interested in two types of solutions. A third one is added for completeness.

Definition 1.6.1. *Let Hypothesis 1.2.1 be valid. Suppose that the operator equation* (1.6) *has the solution $y \in W(0,T)^s$.*

- *Let $y_0 \in L^2(\Omega)^s$. The solution y is called transient (with the initial value y_0) if $y_j(0) = y_{0j}$ for all $j \in \{1, \dots, s\}$.*
- *The solution y is called periodic if $y_j(0) = y_j(T)$ for all $j \in \{1, \dots, s\}$.*

In the context of parameter identification, the solution of a model equation (the "model output") is compared to observational data from the investigated ecosystem (cf. Chapter 5). Available data are often "climatological", i.e., they represent an average over several years. Since periodic solutions correspond to this type of data, they are of particular interest. Transient solutions, on the other hand, correspond to data related to an actual year.

The additional type of stationary solutions reflects the equilibrium concentrations that are reached if the "forcing", caused by velocity, diffusion, reaction terms, and right-hand sides, is constant with respect to time. The characterizing equation is a time-independent variant of the model equation (1.6). In particular, the temporal derivative is equal to zero.

Let $\mathbf{v} \in H^1(\Omega)^{n_d}$ and $\kappa \in L^\infty(\Omega)$. We define the time-independent linear operator $B_{stat}^s : H^1(\Omega)^s \to (H^1(\Omega)^*)^s$ by

$$\langle B_{stat}^s(v), w \rangle := \sum_{j=1}^{s} \left(\int_\Omega (\kappa \nabla v_j \cdot \nabla w_j) dx + \int_\Omega (\mathbf{v} \cdot \nabla v_j) w_j dx \right) \quad \text{for all } v, w \in H^1(\Omega)^s.$$

Moreover, we consider the operator $F_{stat} : \Lambda \to (H^1(\Omega)^*)^s$ and the right-hand side $f_{stat} \in (H^1(\Omega)^*)^s$. A stationary solution $y \in H^1(\Omega)^s \cap \Lambda$ is characterized by solving the equation

$$B^s_{stat}(y) + F_{stat}(y) = f_{stat}. \tag{1.9}$$

A stationary solution in $H^1(\Omega)^s$ can be identified with an element of $W(0,T)^s$. Being constant with respect to time, this element is periodic in the sense that initial and terminal values coincide. However, it is not a periodic solution of the time-dependent equation (1.6) because, unlike periodic solutions, stationary solutions correspond to a constant forcing. Therefore, the existence of stationary solutions does not imply the existence of a constant periodic solution.

Periodic and stationary solutions are closely related as we will see in Chapter 3. As a consequence, the method we develop to prove the existence of periodic solutions applies also to stationary solutions after only slight modifications. Mainly for this reason, we incorporate a result about stationary solutions in this work. In applications, they are less important than transient or periodic solutions because a constant forcing is not realistic.

Chapter 2

Transient solutions for a general model class

2.1 Introduction to the model class

In this chapter, we investigate transient solutions of a specific class of ecosystem models. The class is distinguished by reaction terms containing a monotone and a Lipschitz continuous part. As we will see in Chapter 4, the PO_4-DOP model belongs to this class because all featured reaction terms are Lipschitz continuous.

We prove existence and uniqueness of transient solutions with the help of two different techniques. The first proof relies on Galerkin's method which is a standard approach in connection with transient solutions of partial differential equations. The second proof is based on Banach's Fixed Point Theorem. Evans [5, Section 9.2.1, Theorem 2] uses this technique to solve an initial boundary value problem with purely Lipschitz continuous reaction terms and homogeneous Dirichlet boundary conditions. Following both approaches, we obtain two different existence results, formulated in the theorems 2.2.1 and 2.3.2. The second result, based on Banach's theorem, has the advantage of being constructive. However, its proof relies on a special case of the first result. Since the latter additionally permits a slightly larger domain of definition for the reaction terms, it is worth being stated on its own.

The ideas of both proofs can be found in literature; especially, Galerkin's method has been applied in many variations. Our achievement will consist in adapting the standard methods to the special situation of ecosystem models.

To specify the model class, we need the following fundamental assumptions.

Hypothesis 2.1.1. *Let $f \in L^2(0,T;H^1(\Omega)^*)^s$ and $i \in \{1,2\}$. Suppose that Y_i are Banach spaces with $W(0,T)^s \hookrightarrow Y_i$ and that $\Lambda_i \subseteq L^2(\Omega)^s$ and Y_i fulfill property* (1.1)*. Furthermore, we assume that the operators $F_i : Y_i \to L^2(0,T;H^1(\Omega)^*)^s$ are generated by the indexed families $(F_i(t))_t$ of operators $F_i(t) : \Lambda_i \to (H^1(\Omega)^*)^s$ in the sense of* (1.2).

The model class covered in this chapter is characterized by the operator equation

$$y' + B^s(y) + F_1(y) + F_2(y) = f \quad \text{in } L^2(0,T;H^1(\Omega)^*)^s.$$

The properties of the operators F_1 and F_2 are specified in Theorem 2.2.1 below. The considerations before Equation (1.6) show the connection between the general operators F_1, F_2 and the reaction terms d, b of an ecosystem model.

2.2 An existence and uniqueness result with Galerkin's method

Theorem 2.2.1. *Beside Hypothesis 2.1.1, let $L^2(0,T;H^1(\Omega))^s$ be continuously embedded in Y_2. We assume that the operators F_i are homogeneous, i.e., $F_i(0) = 0$. Suppose that F_2 is demicontinuous and $F_2(t)$ is continuous and monotone, i.e.,*

$$\langle F_2(y(t)) - F_2(v(t)), y(t) - v(t)\rangle \geq 0 \quad \textit{for almost all } t \in [0,T]$$

given $y, v \in L^2(0,T;H^1(\Omega))^s$. Furthermore, $F_1(t)$ satisfies the Lipschitz condition

$$\|F_1(y(t)) - F_1(v(t))\|_{(H^1(\Omega)^*)^s} \leq L_1\|y(t) - v(t)\|_{\Omega^s} \quad \textit{for almost all } t \in [0,T]$$

given $y, v \in L^2(Q_T)^s \cap Y_1$ with $L_1 > 0$ independent of t. Moreover, let one of the conditions

1. *The embedding $W(0,T)^s \hookrightarrow Y := Y_1 \cap Y_2$ is compact;*
2. *$F_2 = 0$ and F_1 is weakly continuous;*
3. *$F_2 \neq 0$ and F_1 is strongly continuous;*

be valid. Then, the initial value problem

$$\begin{aligned} y' + B^s(y) + F_1(y) + F_2(y) &= f \\ y(0) &= y_0 \end{aligned} \tag{2.1}$$

has a unique solution $y \in W(0,T)^s$ for every $y_0 \in L^2(\Omega)^s$.

The proof of Theorem 2.2.1 follows after a proposition about a priori estimates.

Proposition 2.2.2. *Suppose that the operators $F_i : Y_i \to L^2(0,T;H^1(\Omega)^*)^s$ fulfill the assumptions of Theorem 2.2.1. Furthermore, let Z be a closed subspace of $H^1(\Omega)$.*

1. *Let z_1, z_2 be elements of $W(0,T)^s$ in case $Z = H^1(\Omega)$ or else of $H^1(0,T;Z)^s$. Suppose that the difference $z := z_1 - z_2$ fulfills*

$$\langle z'(t), v\rangle + B^s(z,v;t) + \sum_{i=1}^{2}\langle F_i(z_1(t)) - F_i(z_2(t)), v\rangle = \langle f(t), v\rangle \tag{2.2}$$

for all $v \in Z^s$ and almost all $t \in [0,T]$. Here, we define $\langle z'(t), v\rangle := (z'(t), v)_{\Omega^s}$ if $z'(t)$ is a function. Then, there exists a constant $C > 0$ independent of z, f, F_2 with

$$\|z\|_{C([0,T];L^2(\Omega))^s} + \|z\|_{L^2(0,T;H^1(\Omega))^s} \le C(\|f\|_{L^2(0,T;H^1(\Omega)^*)^s} + \|z(0)\|_{L^2(\Omega)^s}).$$

2. *Let $M > 0$. We define the set K_M as a subset of $W(0,T)^s$ in case $Z = H^1(\Omega)$ or else of $H^1(0,T;Z)^s$ as follows: An element z of $W(0,T)^s$ or $H^1(0,T;Z)^s$ belongs to K_M if and only if $\|z(0)\|_{L^2(\Omega)^s} \le M$ and the variant of Equation* (2.2)

$$\langle z'(t), v\rangle + B^s(z, v; t) + \sum_{i=1}^{2} \langle F_i(z(t)), v\rangle = \langle f(t), v\rangle \tag{2.3}$$

holds for all $v \in Z^s$ and almost all $t \in [0,T]$. Then, there exists a constant $M^* > 0$ independent of z with

$$\|z'\|_{L^2(0,T;H^1(\Omega)^*)^s} \le M^* \quad \text{for all } z \in K_M.$$

In case $F_2 = 0$, the derivative of every $z \in W(0,T)^s$ or $z \in H^1(0,T;Z)^s$ satisfying (2.3) *can be estimated by*

$$\|z'\|_{L^2(0,T;H^1(\Omega)^*)^s} \le \tilde{C}\left(\|f\|_{L^2(0,T;H^1(\Omega)^*)^s} + \|z\|_{L^2(0,T;H^1(\Omega))^s}\right)$$

with a constant $\tilde{C} > 0$ independent of z and f.

Proof. Concerning the first assertion, Equation (2.2) implies

$$\langle z'(t), z(t)\rangle + B^s(z, z; t) + \sum_{i=1}^{2} \langle F_i(z_1(t)) - F_i(z_2(t)), z(t)\rangle = \langle f(t), z(t)\rangle \tag{2.4}$$

almost everywhere since $z(t)$ belongs to Z^s for almost all $t \in [0,T]$. First, we observe

$$\langle F_2(z_1(t)) - F_2(z_2(t)), z(t)\rangle = \langle F_2(z_1(t)) - F_2(z_2(t)), z_1(t) - z_2(t)\rangle \ge 0$$

because of the monotonicity assumed for $F_2(t)$. Using additionally Theorem 1.1.2(2), Equation (2.4) leads to the estimate

$$\frac{1}{2}\frac{d}{dt}\|z(t)\|^2_{\Omega^s} + B^s(z, z; t) \le \langle f(t), z(t)\rangle - \langle F_1(z_1(t)) - F_1(z_2(t)), z(t)\rangle.$$

Both of the summands on the right-hand side are estimated by means of Cauchy's inequality with an arbitrary $\varepsilon > 0$ (see, for instance, Evans [5, Appendix B.2]). We obtain for the first summand

$$\langle f(t), z(t)\rangle \le \|f(t)\|_{(H^1(\Omega)^*)^s}\|z(t)\|_{H^1(\Omega)^s} \le \frac{1}{4\varepsilon}\|f(t)\|^2_{(H^1(\Omega)^*)^s} + \varepsilon\|z(t)\|^2_{H^1(\Omega)^s}.$$

Employing the Lipschitz condition, we similarly conclude for the second summand

$$
\begin{aligned}
|\langle F_1(z_1(t)) - F_1(z_2(t)), z(t)\rangle| &\leq \|F_1(z_1(t)) - F_1(z_2(t))\|_{(H^1(\Omega)^*)^s} \|z(t)\|_{H^1(\Omega)^s} \\
&\leq L_1 \|z_1(t) - z_2(t)\|_{\Omega^s} \|z(t)\|_{H^1(\Omega)^s} \leq \frac{L_1^2}{4\varepsilon} \|z(t)\|_{\Omega^s}^2 + \varepsilon \|z(t)\|_{H^1(\Omega)^s}^2. \qquad (2.5)
\end{aligned}
$$

Estimating B^s according to Lemma 1.4.2(2), we arrive at

$$
\begin{aligned}
\frac{1}{2} \frac{d}{dt} \|z(t)\|_{\Omega^s}^2 \leq \frac{1}{4\varepsilon} \|f(t)\|_{(H^1(\Omega)^*)^s}^2 + \varepsilon \|z(t)\|_{H^1(\Omega)^s}^2 + \frac{L_1^2}{4\varepsilon} \|z(t)\|_{\Omega^s}^2 \\
+ \varepsilon \|z(t)\|_{H^1(\Omega)^s}^2 + \kappa_{\min} \|z(t)\|_{\Omega^s}^2 - \kappa_{\min} \|z(t)\|_{H^1(\Omega)^s}^2.
\end{aligned}
$$

We choose $\varepsilon := \kappa_{\min}/4$. Rearranging the summands and gathering the coefficients in $c_1 = 2\kappa_{\min} + 2L_1^2/\kappa_{\min}$, we transform the inequality into

$$
\begin{aligned}
\frac{d}{dt} \|z(t)\|_{\Omega^s}^2 &\leq \frac{1}{2\varepsilon} \|f(t)\|_{(H^1(\Omega)^*)^s}^2 + c_1 \|z(t)\|_{\Omega^s}^2 - 2(\kappa_{\min} - 2\varepsilon) \|z(t)\|_{H^1(\Omega)^s}^2 \\
&\leq \frac{2}{\kappa_{\min}} \|f(t)\|_{(H^1(\Omega)^*)^s}^2 + c_1 \|z(t)\|_{\Omega^s}^2 - \kappa_{\min} \|z(t)\|_{H^1(\Omega)^s}^2 \qquad (2.6) \\
&\leq \frac{2}{\kappa_{\min}} \|f(t)\|_{(H^1(\Omega)^*)^s}^2 + c_1 \|z(t)\|_{\Omega^s}^2.
\end{aligned}
$$

Gronwall's lemma (see, for instance, Evans [5, Appendix B.2]) yields

$$
\begin{aligned}
\|z(t)\|_{\Omega^s}^2 &\leq \mathrm{e}^{tc_1} \left[\|z(0)\|_{\Omega^s}^2 + \int_0^t \frac{2}{\kappa_{\min}} \|f(\sigma)\|_{(H^1(\Omega)^*)^s}^2 d\sigma \right] \qquad (2.7) \\
&\leq C_1 \left[\|z(0)\|_{\Omega^s}^2 + \|f\|_{L^2(0,T;H^1(\Omega)^*)^s}^2 \right]
\end{aligned}
$$

for all $t \in [0,T]$ with $C_1 := \exp(Tc_1) \max\{1, 2/\kappa_{\min}\}$. This yields the desired estimate of the $C([0,T];L^2(\Omega))^s$-norm of z.

To derive an analogous result in $L^2(0,T;H^1(\Omega))^s$, we return to Equation (2.6) and add $\kappa_{\min} \|z(t)\|_{H^1(\Omega)^s}^2$ on both sides of the inequality. Integration with respect to t yields

$$
\int_0^T \frac{d}{dt} \|z(t)\|_{\Omega^s}^2 dt + \kappa_{\min} \|z\|_{L^2(0,T;H^1(\Omega))^s}^2 \leq \int_0^T c_1 \|z(t)\|_{\Omega^s}^2 dt + \frac{2}{\kappa_{\min}} \|f\|_{L^2(0,T;H^1(\Omega)^*)^s}^2.
$$

The first integral is transformed by virtue of Theorem 1.1.2. The integrand on the right-hand side is bounded by the $C([0,T];L^2(\Omega))^s$-norm of z. We conclude

$$
\|z(T)\|_{\Omega^s}^2 + \kappa_{\min} \|z\|_{L^2(0,T;H^1(\Omega))^s}^2 \leq Tc_1 \|z\|_{C([0,T];L^2(\Omega))^s}^2 + \frac{2}{\kappa_{\min}} \|f\|_{L^2(0,T;H^1(\Omega)^*)^s}^2 + \|z(0)\|_{\Omega^s}^2.
$$

The summand $\|z(T)\|_{\Omega^s}^2$ is nonnegative. Using the estimate of the $C([0,T];L^2(\Omega))^s$-norm of z, we obtain

$$
\|z\|_{L^2(0,T;H^1(\Omega))^s}^2 \leq C_2 \left[\|z(0)\|_{\Omega^s}^2 + \|f\|_{L^2(0,T;H^1(\Omega)^*)^s}^2 \right] \qquad (2.8)
$$

with $C_2 := (C_1 T c_1 + \max\{2/\kappa_{\min}, 1\})/\kappa_{\min}$. Combining the square roots of the two estimates for z and estimating the right-hand side using the binomial theorem, we obtain the theorem's first assertion with the constant $C := \sqrt{C_1} + \sqrt{C_2}$.

We proceed with the theorem's second part. Let $z \in K_M$. First, we estimate $F_2(z)$ using Corollary III.1.2 of Gajewski et al. [7]. By assumption, F_2, regarded as an operator from $L^2(0,T;H^1(\Omega))^s$ to $L^2(0,T;H^1(\Omega)^*)^s$, is monotone. Furthermore, Equation (2.8), applied to $z_1 = z$ and $z_2 = 0$, and the condition for the initial value yield

$$\|z\|_{L^2(0,T;H^1(\Omega))^s} \le C_2 \left[\|f\|_{L^2(0,T;H^1(\Omega)^*)^s} + M\right] =: M_1.$$

We use the techniques of the proof of the theorem's first part to show the existence of a constant $M_2 > 0$ with $\langle F_2(z), z\rangle_{L^2(0,T;H^1(\Omega)^*)^s} \le M_2$. Repeating all steps in the transformation of (2.2) into (2.6) except for the estimate of the summand with F_2, we obtain

$$\langle F_2(z(t)), z(t)\rangle \le \frac{2}{\kappa_{\min}}\|f(t)\|^2_{(H^1(\Omega)^*)^s} + c_1\|z(t)\|^2_{\Omega^s} - \frac{d}{dt}\|z(t)\|^2_{\Omega^s}.$$

Integration with respect to t and Theorem 1.1.2 yield

$$\begin{aligned}\langle F_2(z), z\rangle_{L^2(0,T;H^1(\Omega)^*)^s} &\le \frac{2}{\kappa_{\min}}\|f\|^2_{L^2(0,T;H^1(\Omega)^*)^s} + c_1\|z\|^2_{L^2(0,T;L^2(\Omega))^s} - \|z(T)\|^2_{\Omega^s} + \|z(0)\|^2_{\Omega^s}\\ &\le \frac{2}{\kappa_{\min}}\|f\|^2_{L^2(0,T;H^1(\Omega)^*)^s} + c_1 M_1^2 + M^2 =: M_2.\end{aligned}$$

The constants M_1 and M_2 are independent of z. Thus, the corollary of Gajewski et al. provides a constant M_F with

$$\|F_2(z)\|_{L^2(0,T;H^1(\Omega)^*)^s} \le M_F \quad \text{for all } z \in K_M. \tag{2.9}$$

To prove the proposition's second statement, let $v \in H^1(\Omega)^s$ with $\|v\|_{H^1(\Omega)^s} = 1$. First, we express $\langle z'(t), v\rangle$ by means of Equation (2.3). To this end, we write $v = v_1 + v_2$ with $v_1 \in Z^s$ and $v_2 \in (Z^s)^\perp$. This representation of v exists because Z is a closed subset of $H^1(\Omega)$.

In case $Z \ne H^1(\Omega)$, the derivative $z'(t)$ belongs to Z^s and is thus orthogonal to v_2 in $H^1(\Omega)^s$. This implies $(z'(t), v_2)_{\Omega^s} = 0$ because $L^2(\Omega)^s$ and $H^1(\Omega)^s$ have a simultaneous orthogonal basis (see, for instance, Evans [5, Section 7.1.2]). Furthermore, $v_1 \in Z^s$ is admitted as a test function in Equation (2.3). We conclude

$$\langle z'(t), v\rangle = (z'(t), v)_{\Omega^s} = (z'(t), v_1)_{\Omega^s} = \langle f(t), v_1\rangle - B^s(z, v_1; t) - \sum_{i=1}^{2}\langle F_i(z(t)), v_1\rangle$$

for almost all $t \in [0,T]$. The same equation holds if $Z^s = H^1(\Omega)^s$. In this case, $v_2 = 0$, and $v = v_1 \in H^1(\Omega)^s$ itself is admitted as a test function in (2.3).

In the next step, we estimate the right-hand side of the equation for $\langle z'(t), v\rangle$. Since

$F_1(0) = 0$, the Lipschitz continuous summand can be estimated by

$$\langle F_1(z(t)) - F_1(0), v_1 \rangle \leq L_1 \|z(t)\|_{\Omega^s} \|v_1\|_{H^1(\Omega)^s} \leq L_1 \|z(t)\|_{H^1(\Omega)^s} \|v_1\|_{H^1(\Omega)^s}. \tag{2.10}$$

Similar estimates hold for the summands including $f(t)$ and $F_2(z(t))$. Lemma 1.4.2(1) provides an estimate for B^s. Furthermore, the orthogonality of v_1 and v_2 in combination with the Pythagorean theorem in the Hilbert space $H^1(\Omega)^s$ yields

$$\|v_1\|^2_{H^1(\Omega)^s} \leq \|v_1\|^2_{H^1(\Omega)^s} + \|v_2\|^2_{H^1(\Omega)^s} = \|v\|^2_{H^1(\Omega)^s} = 1.$$

Finally, the norm in $L^2(\Omega)^s$ is bounded by the norm in $H^1(\Omega)^s$. We conclude

$$\begin{aligned} \|z'(t)\|^2_{(H^1(\Omega)^*)^s} = \sup_{\|v\|=1} \langle z'(t), v\rangle^2 &\leq \left(\|f(t)\|_{(H^1(\Omega)^*)^s} + C_3\|z(t)\|_{H^1(\Omega)^s} + \|F_2(z(t))\|_{(H^1(\Omega)^*)^s}\right)^2 \\ &\leq 3\left(\|f(t)\|^2_{(H^1(\Omega)^*)^s} + C_3^2\|z(t)\|^2_{H^1(\Omega)^s} + \|F_2(z(t))\|^2_{(H^1(\Omega)^*)^s}\right) \end{aligned}$$

with $C_3 := C_B + L_1$. The last estimate is valid because of the convexity of the square function on $\mathbb{R}$. We integrate this estimate with respect to t and insert the upper bounds derived for z and $F_2(z)$. The result is

$$\begin{aligned} \|z'\|^2_{L^2(0,T;H^1(\Omega)^*)^s} &\leq 3(\|f\|^2_{L^2(0,T;H^1(\Omega)^*)^s} + C_3^2\|z\|^2_{L^2(0,T;H^1(\Omega))^s} + \|F_2(z)\|^2_{L^2(0,T;H^1(\Omega)^*)^s}) \\ &\leq 3(\|f\|^2_{L^2(0,T;H^1(\Omega)^*)^s} + C_3^2 M_1^2 + M_F^2) =: M^{*2}. \end{aligned}$$

We obtain the proposition's second assertion by extracting the square root.

The additional statement about equations with purely Lipschitz continuous operators is a consequence of the first line of the last estimate. The norm of $F_2(z)$ vanishes in this case. □

Proof of Theorem 2.2.1. Let $y_0 \in L^2(\Omega)^s$. Choose an orthogonal basis $(v_j)_{j\in\mathbb{N}}$ of the separable Hilbert space $H^1(\Omega)$. It can be considered an orthonormal basis of $L^2(\Omega)$ after a possible orthonormalization (cf. Evans [5, Section 7.1.2]).

We will approximate the desired solution by a sequence $(y_n)_n$ consisting of the members $y_n = (y_{1n}, \ldots, y_{sn})$. Let $n \in \mathbb{N}$. For every $l \in \{1, \ldots, s\}$, the l-th component of the sequence's n-th member belongs to the finite-dimensional subspace $\operatorname{span}\{v_1, \ldots, v_n\}$ of $H^1(\Omega)$ and is described by the ansatz

$$y_{ln}(t) = \sum_{i=1}^{n} {}^l u_i^n(t) v_i$$

at every point of time t. We will determine the coefficients

$$u^n : [0,T] \to \mathbb{R}^{n\times s} \quad \text{with} \quad u^n = \begin{pmatrix} {}^1u_1^n & \cdots & {}^su_1^n \\ \vdots & \ddots & \vdots \\ {}^1u_n^n & \cdots & {}^su_n^n \end{pmatrix}$$

in such a way that $y_{ln}(t)$ solves

$$(y'_{ln}(t), v_j)_\Omega + B(y_{ln}, v_j; t) + \sum_{m=1}^{2} \langle F_{ml}(y_n(t)), v_j \rangle_{H^1(\Omega)^*} = \langle f_l(t), v_j \rangle_{H^1(\Omega)^*} \tag{2.11}$$

and that $(y_{0l}, v_j)_\Omega = (y_{ln}(0), v_j)_\Omega$ holds for all $j \leq n$ and all $l \leq s$.

We insert the ansatz for $y_{ln}(t)$ into (2.11). The linearity of the first two summands and the orthonormality of the basis yield for the left-hand side of the equation

$$\begin{aligned}(\sum_{i=1}^{n} {}^l u_i^{n\prime}(t) v_i, v_j)_\Omega + B(\sum_{i=1}^{n} {}^l u_i^n(t) v_i, v_j; t) + \sum_{m=1}^{2} \langle F_{ml}((\sum_{i=1}^{n} {}^k u_i^n(t) v_i)_{k \leq s}), v_j \rangle_{H^1(\Omega)^*} \\ = {}^l u_j^{n\prime}(t) + \sum_{i=1}^{n} {}^l u_i^n(t) B(v_i, v_j; t) + \Phi_{jl}(t, u^n(t)).\end{aligned}$$

Here, we gather the last two terms in a function of the coefficient matrix u^n, namely

$$\Phi_{jl}(t, u^n(t)) := \sum_{m=1}^{2} \langle F_{ml}((\sum_{i=1}^{n} {}^k u_i^n(t) v_i)_{k \leq s}), v_j \rangle_{H^1(\Omega)^*}.$$

The same arguments yield $(y_{0l}, v_j)_\Omega = (y_{ln}(0), v_j)_\Omega = (\sum_{i=1}^{n} {}^l u_i^n(0) v_i, v_j)_\Omega = {}^l u_j^n(0)$ for the initial value.

Combining these equations for all $j \leq n$ and $l \leq s$, we observe that the coefficient matrix u^n solves the $(n \times s)$-dimensional nonlinear system of ordinary differential equations

$$\begin{aligned}\frac{d}{dt} u^n(t) &= r(t) - A(t) u^n(t) - \Phi(t, u^n(t)) \\ u^n(0) &= ((y_{0l}, v_j)_\Omega)_{\substack{j=1,\ldots,n,\\ l=1,\ldots,s}}.\end{aligned} \tag{2.12}$$

Here, we use the abbreviations

$$\Phi := (\Phi_{jl})_{\substack{j=1,\ldots,n,\\ l=1,\ldots,s}} : [0,T] \times \mathbb{R}^{n \times s} \to \mathbb{R}^{n \times s}, \quad r := (\langle f_l(\,.\,), v_j \rangle)_{\substack{j=1,\ldots,n,\\ l=1,\ldots,s}} : [0,T] \to \mathbb{R}^{n \times s}$$

and $A := (B(v_i, v_j; .))_{\substack{j=1,\ldots,n,\\ i=1,\ldots,n}} \in L^2(0,T)^{n \times n}$. In each case, the index above counts the number of lines.

We prove the solvability of (2.12) after stating an a priori estimate for an absolutely continuous solution $u^n \in H^1(0,T)^{n \times s}$. If the entries of the vector $y_n = (y_{1n}, \ldots, y_{sn})$ are defined by the ansatz with the coefficients u^n, the orthonormality of $(v_j)_{j \in \mathbb{N}}$ in $L^2(\Omega)$ yields

$$\|y_n(t)\|_{\Omega^s}^2 = \sum_{l=1}^{s} \| \sum_{i=1}^{n} {}^l u_i^n(t) v_i \|_\Omega^2 = \sum_{l=1}^{s} \sum_{i=1}^{n} {}^l u_i^n(t)^2 = \|u^n(t)\|_{\mathbb{R}^{n \times s}}^2.$$

Thus, an a priori estimate for y_n provides an estimate for u^n as well.

An estimate for y_n follows from Proposition 2.2.2, applied to the finite-dimensional and therefore closed subspace $Z := \operatorname{span}\{v_1, \ldots, v_n\}$ of $H^1(\Omega)$ and the set $K_M := \{y_n\}$.

We show that K_M fulfills the assumptions of the proposition's second part. Since the coefficient matrix u^n belongs to $H^1(0,T)^{n\times s}$, the associated ansatz function y_n is an element of $H^1(0,T;Z)^s$. To obtain an equivalent of (2.3), we use that all elements of Z are linear combinations of $v_1, \ldots, v_n$. We multiply the equations (2.11), which are equivalent to (2.12), by an arbitrary constant c_{jl} and summate across $j \in \{1, \ldots, n\}$ and $l \in \{1, \ldots, s\}$. Furthermore, the initial value $y_n(0)$ is bounded by $M := \|y_0\|_{\Omega^s}$. This is shown by the initial value condition in (2.12), the orthonormality of the basis elements and Bessel's inequality. These arguments enable the estimate

$$\begin{aligned} \|y_n(0)\|_{\Omega^s}^2 &= \sum_{l=1}^{s} \| \sum_{i=1}^{n} {}^l u_i^n(0) v_i\|_\Omega^2 = \sum_{l=1}^{s} \| \sum_{i=1}^{n} (y_{0l}, v_i)_\Omega v_i\|_\Omega^2 = \sum_{l=1}^{s} \sum_{i=1}^{n} (y_{0l}, v_i)_\Omega^2 \\ &\le \sum_{l=1}^{s} \|y_{0l}\|_\Omega^2 = \|y_0\|_{\Omega^s}^2. \end{aligned} \tag{2.13}$$

Thus, both parts of Proposition 2.2.2 yield an upper bound $M_{up} > 0$ independent of y_n such that

$$\sup_{t\in[0,T]} \|y_n(t)\|_{\Omega^s} + \|y_n\|_{W(0,T)^s} \le M_{up}. \tag{2.14}$$

Note that the considerations above remain valid for the set $K_M := \{y_{\tilde{n}} : \tilde{n} \in \mathbb{N}\}$. Thus, (2.14) holds for every member of the sequence $(y_{\tilde{n}})_{\tilde{n}\in\mathbb{N}}$ and M_{up} is independent of $\tilde{n}$.

In particular, we obtain the a priori estimate $\|u^n(t)\|_{\mathbb{R}^{n\times s}} \le M_{up}$ for each solution of (2.12) on a subinterval of $[0,T]$.

The existence of a solution u^n of (2.12) on $[0,T]$ follows from Problem 30.2(iv) in Zeidler [29], proved by means of the existence theorem of Carathéodory (cf. Coddington and Levinson [3, Theorem 2.1.1]). To apply this result, we define the compact set $K := \{u^n \in \mathbb{R}^{n\times s} : \|u^n\|_{\mathbb{R}^{n\times s}} \le 2M_{up}\}$. First, we prove that the right-hand side

$$R : [0,T] \times K \to \mathbb{R}^{n\times s}, \quad R(t,u^n) := r(t) - A(t)u^n - \Phi(t,u^n)$$

satisfies the Carathéodory condition. Clearly, $t \mapsto r(t) - A(t)u^n - \Phi(t,u^n)$ is measurable for every $u^n \in K$. Furthermore, $u^n \mapsto r(t) - A(t)u^n - \Phi(t,u^n)$ is continuous for almost every $t \in [0,T]$. This is the case because the linear summand is given by a matrix multiplication and $u^n \mapsto \Phi(t,u^n)$ is a composition of continuous functions. The component $F_2(t)$ is continuous by assumption, and the continuity of $F_1(t)$ is a consequence of the Lipschitz condition.

Finally, let $u^n \in K$. We prove that the norm of $R(\,.\,,u^n)$ is bounded by a Lebesgue-integrable function. The upper bound in

$$\|r(t) - A(t)u^n\|_{\mathbb{R}^{n\times s}} \le \|r(t)\|_{\mathbb{R}^{n\times s}} + \|A(t)\|_{\mathbb{R}^{n\times n}} 2M_{up}$$

is integrable with respect to t since this is true for r and all entries $B(v_i, v_j; .)$ of the matrix $A(.)$. The two summands of $\Phi(\,.\,, u^n)$ are estimated separately. Referring to the ansatz function belonging to u^n as y_n, we estimate the (j,l)-th entry of the first summand $\langle F_{1l}(t)(y_n), v_j \rangle_{H^1(\Omega)^*}$ for almost every t by means of the Lipschitz condition, the homogeneity of F_1, and the fact that $y_n(t)$ and $u^n(t)$ have the same norm. Since u^n belongs to K, we obtain the upper bound $2L_1 M_{up} \|v_j\|_{H^1(\Omega)}$, which is constant and therefore integrable with respect to t.

For almost every t, we regard the (j,l)-th entry of the second summand as the function $f_t : K \to \mathbb{R}$, $f_t(u_n) = \langle F_{2l}(t)(y_n), v_j \rangle_{H^1(\Omega)^*}$ using again the abbreviation y_n for the ansatz function belonging to u^n. We have already shown that the function f_t is continuous. Furthermore, f_t maps the compact set K into $\mathbb{R}$ and thus has a minimum at $u^n_{\min}(t) \in K$ and a maximum at $u^n_{\max}(t) \in K$. It remains to be shown that the upper bound in

$$|f_t(u^n)| \leq \max\{|f_t(u^n_{\min}(t))|, |f_t(u^n_{\max}(t))|\}$$

is integrable with respect to t. Since $u^n_{\min}(t)$ belongs to K, the corresponding ansatz function $y_{n,\min}$ is an element of $L^2(0,T;H^1(\Omega))^s$ and therefore also of the domain of definition Y_2 of F_2. As a consequence, $F_2(y_{n,\min})$ lies in $L^2(0,T;H^1(\Omega)^*)^s$. Thus, a standard estimate yields that $f_t(u^n_{\min}(.))$ is integrable with respect to t. The same holds for $f_t(u^n_{\max}(.))$.

Thus, all assumptions of Problem 30.2 of Zeidler [29] are fulfilled. It provides a solution of (2.12) which is absolutely continuous on $[0,T]$ and fulfills (2.12) almost everywhere.

For every $n \in \mathbb{N}$, let $y_n \in W(0,T)^s$ be the ansatz function associated with the solution u^n of (2.12). Since the a priori estimate (2.14) holds for all $n \in \mathbb{N}$ and the upper bound is independent of n, the sequence $(y_n)_{n\in\mathbb{N}}$ is bounded in $W(0,T)^s$ which is a Hilbert space and thus reflexive. The theorem of Eberlein-Shmulyan (see, for instance, Yosida [27, Appendix to Chapter V]) yields a subsequence $(y_{n_k})_{k\in\mathbb{N}}$ and a limit $y \in W(0,T)^s$ with $y_{n_k} \rightharpoonup y$ in $L^2(0,T;H^1(\Omega))^s$ and $y'_{n_k} \rightharpoonup y'$ in $L^2(0,T;H^1(\Omega)^*)^s$ for $k \to \infty$.

The ansatz functions y_{n_k} fulfill Equation (2.11) for almost every $t \in [0,T]$. To transform (2.11) into an operator equation in $L^2(0,T;H^1(\Omega)^*)^s$, we choose $m \in \mathbb{N}$ and arbitrary smooth functions $d_{jl} : [0,T] \to \mathbb{R}$ for all $j \in \{1,\ldots,m\}$, $l \in \{1,\ldots,s\}$. We multiply (2.11) by the corresponding coefficient $d_{jl}(t)$, summate across $j \in \{1,\ldots,m\}$ and $l \in \{1,\ldots,s\}$, and integrate with respect to t. We obtain

$$\int_0^T \{\langle y'_{n_k}(t), w(t)\rangle + B^s(y_{n_k}, w; t) + \langle F(y_{n_k}(t)), w(t)\rangle\} dt = \int_0^T \langle f(t), w(t)\rangle dt \qquad (2.15)$$

with the special test function $w \in C^\infty([0,T];H^1(\Omega))^s$ defined by the components

$$w_l = \sum_{j=1}^m d_{jl} v_j \in C^\infty([0,T];H^1(\Omega)) \quad \text{for all } l \in \{1,\ldots,s\}. \qquad (2.16)$$

Functions of this type lie dense in $L^2(0,T;H^1(\Omega))^s$ since $(v_j)_{j\in\mathbb{N}}$ is a basis of $H^1(\Omega)$ and the space of smooth functions is dense in the space of quadratically integrable functions, see Rudin [21, Theorem 3.14] and Emmrich [4, Theorem 8.1.9]. Thus, Equation (2.15) holds for all $w \in L^2(0,T;H^1(\Omega))^s$ and all $k \in \mathbb{N}$.

Equation (2.15) and the considerations concerning the test functions reveal that each y_{n_k} solves the operator equation in (2.1). To prove that the same is true for the limit y, we investigate the convergence of the summands on the left-hand side of (2.15).

Since, in particular, the sequence of the l-th components $(y_{l n_k})_{k\in\mathbb{N}}$ converges weakly with respect to the norm of $L^2(0,T;H^1(\Omega))$ for every $l \in \{1,\dots,s\}$, we conclude for an arbitrary $w \in L^2(0,T;H^1(\Omega))^s$

$$\int_0^T (\kappa(t)\nabla y_{l n_k}(t), \nabla w_l(t))_{L^2(\Omega)^{n_d}} dt \to \int_0^T (\kappa(t)\nabla y_l(t), \nabla w_l(t))_{L^2(\Omega)^{n_d}} dt \quad \text{and}$$
$$\int_0^T (\mathbf{v}(t)\cdot\nabla y_{l n_k}(t), w_l(t))_{L^2(\Omega)} dt \to \int_0^T (\mathbf{v}(t)\cdot\nabla y_l(t), w_l(t))_{L^2(\Omega)} dt$$

and thus $\langle B^s(y_{n_k}), w\rangle_{L^2(0,T;H^1(\Omega)^*)^s} \to \langle B^s(y), w\rangle_{L^2(0,T;H^1(\Omega)^*)^s}$ if $k\to\infty$. The weak convergence $y'_{n_k} \rightharpoonup y'$ implies

$$\int_0^T \langle y'_{n_k}(t), w(t)\rangle dt \to \int_0^T \langle y'(t), w(t)\rangle dt \quad \text{for all } w \in L^2(0,T;H^1(\Omega))^s.$$

Analogous results for the operators F_1 and F_2 depend on the properties of $Y = Y_1 \cap Y_2$.

Let us first consider the case that $W(0,T)^s$ is compactly embedded in Y. Then, the bounded sequence $(y_{n_k})_k$ has a subsequence, denoted again by $(y_{n_k})_k$, converging strongly in Y and therefore in both Y_1 and Y_2. Since strong convergence implies weak convergence and the weak limit is unique, the strong and the weak limit are both equal to y. The operator F_1 is continuous due to the assumed Lipschitz condition and thus, in particular, demicontinuous. Since F_2 is demicontinuous as well, we obtain for the sum $F := F_1 + F_2$

$$\int_0^T \langle F(y_{n_k}(t)), w(t)\rangle dt \to \int_0^T \langle F(y(t)), w(t)\rangle dt \quad \text{for all } w \in L^2(0,T;H^1(\Omega))^s. \tag{2.17}$$

In summary, we conclude from (2.15)

$$\int_0^T \{\langle y'(t), w(t)\rangle + B^s(y,w;t) + \langle F(y(t)), w(t)\rangle\} dt = \int_0^T \langle f(t), w(t)\rangle dt$$

for all $w \in L^2(0,T;H^1(\Omega))^s$. Thus, in the first case, the proof is complete.

Now we consider the case that the embedding $W(0,T)^s \hookrightarrow Y$ is not compact.

In the purely Lipschitz continuous case ($F_2 = 0$), the assumed weak continuity of F_1 yields $F_1(y_{n_k}) \rightharpoonup F_1(y)$ in $L^2(0,T;H^1(\Omega)^*)^s$. This is true because $W(0,T)^s$ is continuously embedded in Y_1 and thus $(y_{n_k})_k$ converges weakly to y in Y_1. Hence, we obtain a result analogous to (2.17), and the proof is complete.

At last, we consider the case that $F_2 \neq 0$ and F_1 is strongly continuous. Since, in particular, F_1 is weakly continuous, the weak convergence $F_1(y_{n_k}) \rightharpoonup F_1(y)$ is deduced as in the last paragraph. To deduce an analogous result for $F_2 : Y_2 \to L^2(0,T;H^1(\Omega)^*)^s$, we recall that the set $K_M := \{y_{n_k} : k \in \mathbb{N}\}$ fulfills the assumptions of Proposition 2.2.2. Thus, an equivalent of Equation (2.9) holds, i.e., there exists a constant M_F with $\|F_2(y_{n_k})\|_{L^2(0,T;H^1(\Omega)^*)^s} \leq M_F$ for all $k \in \mathbb{N}$. This estimate yields a subsequence, again denoted by $(F_2(y_{n_k}))_k$, and a limit $D \in L^2(0,T;H^1(\Omega)^*)^s$ with $F_2(y_{n_k}) \rightharpoonup D$ in $L^2(0,T;H^1(\Omega)^*)^s$. By passing to limits in (2.15), we obtain

$$\int_0^T \{\langle y'(t), w(t)\rangle + B^s(y,w;t) + \langle D(t), w(t)\rangle\}dt = \int_0^T \langle f(t) - F_1(y(t)), w(t)\rangle dt \tag{2.18}$$

for all $w \in L^2(0,T;H^1(\Omega))^s$.

The proof is finished if $F_2(y) = D$ holds. Following Tröltzsch [26], we establish this identity by means of a lemma from monotone operator theory.

In addition, we will utilize the following lemma about the sequence $(y_{n_k})_k$.

Lemma 2.2.3. *Let $t \in [0,T]$. Then, $(y_{n_k}(t))_k$ converges weakly to $y(t)$ in $L^2(\Omega)^s$. Moreover, the sequence $(y_{n_k}(0))_k$ converges strongly to the initial value $y_0 \in L^2(\Omega)^s$. In particular, the initial value condition $y(0) = y_0$ is satisfied.*

Proof. The operator $E_t : C([0,T];L^2(\Omega))^s \to L^2(\Omega)^s, y \mapsto y(t)$ is obviously linear and bounded due to $\|E_t y\|_{\Omega^s} = \|y(t)\|_{\Omega^s} \leq \sup_{\tau\in[0,T]} \|y(\tau)\|_{\Omega^s} = \|y\|_{C([0,T];L^2(\Omega))^s}$ and thus continuous. Hence, it is also weakly sequentially continuous, see e.g. Tröltzsch [26, Section 2.4.2]. Furthermore, $(y_{n_k})_k$ converges weakly to y in $C([0,T];L^2(\Omega))^s$ because of Theorem 1.1.2(1). The weak sequential continuity of E_t yields the first statement of the lemma.

To prove the second assertion, we consider the ansatz for $y_{l n_k}(0)$ and the Fourier representation $y_{0l} = \sum_{i=1}^{\infty}(y_{0l}, v_i)_\Omega v_i$ of y_{0l} in $L^2(\Omega)$ for every $l \in \{1,\ldots,s\}$. We estimate their difference by using the properties of inner products and orthonormal bases as in (2.13) as well as the initial value condition in (2.12). The convergence in the last step results from the quadratic summability of the Fourier coefficients. We obtain

$$\begin{aligned}
\|y_{n_k}(0) - y_0\|_{\Omega^s}^2 &= \sum_{l=1}^{s} \| \sum_{i=1}^{n_k} {}^l u_i^{n_k}(0) v_i - \sum_{i=1}^{\infty}(y_{0l}, v_i)_\Omega v_i\|_\Omega^2 = \sum_{l=1}^{s} \| \sum_{i=n_k+1}^{\infty} (y_{0l}, v_i)_\Omega v_i\|_\Omega^2 \\
&= \sum_{l=1}^{s} \sum_{i=n_k+1}^{\infty} (y_{0l}, v_i)_\Omega^2 \to 0 \quad \text{for } k \to \infty.
\end{aligned}$$

Finally, $y_{n_k}(0) \to y_0$ in $L^2(\Omega)^s$ implies the weak convergence $y_{n_k}(0) \rightharpoonup y_0$. On the other hand, the first part of the lemma states $y_{n_k}(0) \rightharpoonup y(0)$. The uniqueness of the weak limit yields $y(0) = y_0$. ☐

Now we are able to prove the identity $D = F_2(y)$ in the space $L^2(0,T;H^1(\Omega)^*)^s$. As announced above, we use the following lemma of Gajewski et al. [7, Lemma III.1.3] about monotone operators.

Lemma 2.2.4. *Suppose that the Banach space H is reflexive and that the operator $A : H \to H^*$ is monotone and demicontinuous. Let there be $y, y_n \in H$ for all $n \in \mathbb{N}$ and $w \in H^*$ with the properties $y_n \rightharpoonup y$ in H as well as*

$$(i) \quad A(y_n) \rightharpoonup w \quad \text{in } H^* \quad \text{and} \quad (ii) \quad \limsup_{n\to\infty} \langle A(y_n), y_n \rangle_{H^*} \leq \langle w, y \rangle_{H^*}.$$

Hence, $A(y) = w$ in H^*.

To be conform with the notation of Lemma 2.2.4, we restrict F_2 to $H := L^2(0, T; H^1(\Omega))^s$. This is possible because H is assumed to be continuously embedded in Y_2. In addition, we regard (2.18) as the operator equation

$$y' + w = R(y) \tag{2.19}$$

where the functional $w \in H^*$ and the operator $R : Y_1 \to H^*$ are defined by

$$\langle w, v \rangle_{H^*} := \int_0^T \{B^s(y, v; t) + \langle D(t), v(t) \rangle\} dt \quad \text{and}$$
$$\langle R(\tilde{y}), v \rangle_{H^*} := \int_0^T \{\langle f(t), v(t) \rangle - \langle F_1(\tilde{y}(t)), v(t) \rangle\} dt$$

for all $v \in H, \tilde{y} \in Y_1$. Moreover, we introduce the operator $A : H \to H^*$ with

$$\langle A(\tilde{y}), v \rangle_{H^*} := \int_0^T \{B^s(\tilde{y}, v; t) + \langle F_2(\tilde{y}(t)), v(t) \rangle\} dt \quad \text{for all } \tilde{y}, v \in H.$$

To be able to apply Lemma 2.2.4 to A and w, we check the assumptions. Since $F_2 : Y_2 \to L^2(0, T; H^1(\Omega)^*)^s$ is assumed to be monotone and demicontinuous, these properties remain valid for the operator's restriction to H. Lemma 1.4.2(5) states the monotonicity of B^s and 1.4.2(1) the continuity since B^s is linear. As a consequence, the sum A is monotone and demicontinuous on H.

We have already seen that the sequence $(y_{n_k})_k$ converges weakly to y in H and that $A(y_{n_k}) \rightharpoonup w$ in H^*, i.e., property (i) holds. To verify property (ii), we deduce

$$\int_0^T \langle y'_{n_k}(t), y_{n_k}(t) \rangle dt + \langle A(y_{n_k}), y_{n_k} \rangle_{H^*} = \langle R(y_{n_k}), y_{n_k} \rangle_{H^*}$$

from (2.11) (with n_k instead of n) by multiplying this equation by the coefficient ${}^l u_j^{n_k}(t)$, summating across $l \in \{1, \ldots, s\}$ and $j \in \{1, \ldots, n_k\}$, and integrating with respect to t. Applying Theorem 1.1.2(3) to the integral on the left-hand side and rearranging the summands, we obtain

$$\langle A(y_{n_k}), y_{n_k} \rangle_{H^*} = \langle R(y_{n_k}), y_{n_k} \rangle_{H^*} + \frac{1}{2} \|y_{n_k}(0)\|^2_{\Omega^s} - \frac{1}{2} \|y_{n_k}(T)\|^2_{\Omega^s}. \tag{2.20}$$

Lemma 2.2.3, applied to $t = T$, yields $y_{n_k}(T) \rightharpoonup y(T)$ in $L^2(\Omega)^s$ which implies $\|y(T)\|_{\Omega^s} \leq \liminf_{n\to\infty} \|y_{n_k}(T)\|_{\Omega^s}$ (see, for instance, Yosida [27, Theorem V.1.1(ii)]). Since the upper limit of a real sequence is always greater or equal to the lower limit, we deduce

$$-\limsup_{k\to\infty} \|y_{n_k}(T)\|^2_{\Omega^s} \leq -\liminf_{k\to\infty} \|y_{n_k}(T)\|^2_{\Omega^s} \leq -\|y(T)\|^2_{\Omega^s}.$$

Furthermore, Lemma 2.2.3 implies $\lim_{k\to\infty} \|y_{n_k}(0)\|^2_{\Omega^s} = \|y(0)\|^2_{\Omega^s}$.

Now we investigate the convergence of $\langle R(y_{n_k}), y_{n_k}\rangle_{H^*}$. Since $f \in H^*$ and $(y_{n_k})_k$ converges weakly in H, we conclude $\langle f, y_{n_k}\rangle_{H^*} \to \langle f, y\rangle_{H^*}$ for $k \to \infty$. Moreover, we obtain for the second part of R

$$\begin{aligned}|\langle F_1(y_{n_k}), y_{n_k}\rangle_{H^*} - \langle F_1(y), y\rangle_{H^*}| &\leq |\langle F_1(y_{n_k}) - F_1(y), y_{n_k}\rangle_{H^*}| + |\langle F_1(y), y_{n_k} - y\rangle_{H^*}| \\ &\leq \|F_1(y_{n_k}) - F_1(y)\|_{H^*}\|y_{n_k}\|_H + |\langle F_1(y), y_{n_k} - y\rangle_{H^*}|.\end{aligned}$$

Since $F_1(y) \in H^*$, the hindmost summand converges to zero. The same is true for the first summand because $F_1 : Y_1 \to H^*$ is strongly continuous and $(y_{n_k})_k$ converges weakly in Y_1. In addition, the weakly convergent sequence $(y_{n_k})_k$ is bounded in H. Thus, we conclude $\langle R(y_{n_k}), y_{n_k}\rangle_{H^*} \to \langle R(y), y\rangle_{H^*}$ for $k \to \infty$.

Using these results, we obtain for the upper limit of (2.20)

$$\begin{aligned}\limsup_{k\to\infty}\langle A(y_{n_k}), y_{n_k}\rangle_{H^*} &= \lim_{k\to\infty}\left(\langle R(y_{n_k}), y_{n_k}\rangle_{H^*} + \frac{1}{2}\|y_{n_k}(0)\|^2_{\Omega^s}\right) - \frac{1}{2}\limsup_{k\to\infty}\|y_{n_k}(T)\|^2_{\Omega^s} \\ &\leq \langle R(y), y\rangle_{H^*} + \frac{1}{2}\|y(0)\|^2_{\Omega^s} - \frac{1}{2}\|y(T)\|^2_{\Omega^s} \\ &= \langle R(y), y\rangle_{H^*} - \int_0^T \langle y'(t), y(t)\rangle dt = \langle R(y), y\rangle_{H^*} - \langle y', y\rangle_{H^*} = \langle w, y\rangle_{H^*}.\end{aligned}$$

In the last line, we apply again Theorem 1.1.2(3). The last equality sign is valid because $y \in H$ is both a solution and a proper test function of the operator equation (2.19).

Thus, Lemma 2.2.4 yields $A(y) = w$, i.e.,

$$\int_0^T \{B^s(y, v; t) + \langle F_2(y(t)), v(t)\rangle\}dt = \int_0^T \{B^s(y, v; t) + \langle D(t), v(t)\rangle\}dt \quad \text{for all } v \in H.$$

By subtracting the linear summand on both sides, we obtain $D = F_2(y)$ in H^*, and the proof of existence is complete.

To prove uniqueness, let $y_1, y_2 \in W(0,T)^s$ be two solutions of the initial value problem (2.1). We show that the difference $y := y_1 - y_2$ is equal to zero. Since both y_1 and y_2 have the same initial value, we obtain $y(0) = y_1(0) - y_2(0) = y_0 - y_0 = 0$. The difference of the equations for $y_1(t)$ and $y_2(t)$, endowed with an arbitrary test function $v \in H^1(\Omega)^s$, is equal to

$$\langle y'(t), v\rangle + B^s(y, v; t) + \langle F_1(y_1(t)) - F_1(y_2(t)), v\rangle + \langle F_2(y_1(t)) - F_2(y_2(t)), v\rangle = 0$$

for almost all $t \in [0, T]$. Thus, the assumptions of the first part of Proposition 2.2.2 with $Z = H^1(\Omega)$, $f = 0$, and $z_i = y_i \in W(0,T)^s$ are fulfilled. The proposition yields

$$\|y_1 - y_2\|_{L^2(0,T;H^1(\Omega))^s} \leq C(\|0\|_{L^2(0,T;H^1(\Omega)^*)^s} + \|y(0)\|_{\Omega^s}) = 0.$$

We immediately conclude $y_1 - y_2 = 0$. □

2.3 An existence and uniqueness result with Banach's Fixed Point Theorem

In this section, we prove a second result about existence and uniqueness of transient solutions for the regarded model class. The assumptions about Y_1 are slightly stricter than in Theorem 2.2.1 whereas the operator F_1 is only required to be Lipschitz continuous even if $W(0,T)^s$ is not compactly embedded in $Y_1 \cap Y_2$. Moreover, the proof, based on Banach's Fixed Point Theorem, is constructive. We cite this important theorem below. The proof can be found in Zeidler [28, Theorem 1.A].

Theorem 2.3.1. (Banach) *Let X be a Banach space and the map $A : X \to X$ be Lipschitz continuous with a constant $L \in (0,1)$. Hence, a unique fixed point of A exists in X, i.e., there is $x^* \in X$ with the property $A(x^*) = x^*$.*

The rest of this section is dedicated to the existence theorem and its proof.

Theorem 2.3.2. *Beside Hypothesis 2.1.1, we assume that $C([0,T]; L^2(\Omega))^s \hookrightarrow Y_1$ and $L^2(0,T;H^1(\Omega))^s \hookrightarrow Y_2$ hold. Let the operators F_i be homogeneous, i.e., $F_i(0) = 0$. Suppose that F_2 is demicontinuous and that $F_2(t)$ is continuous and monotone, i.e.*

$$\langle F_2(y(t)) - F_2(v(t)), y(t) - v(t)\rangle \geq 0 \quad \textit{for almost all } t \in [0,T],$$

given $y, v \in L^2(0,T;H^1(\Omega))^s$. Furthermore, $F_1(t)$ satisfies the Lipschitz condition

$$\|F_1(y(t)) - F_1(v(t))\|_{(H^1(\Omega)^*)^s} \leq L_1 \|y(t) - v(t)\|_{\Omega^s} \quad \textit{for almost all } t \in [0,T],$$

given $y, v \in C([0,T]; L^2(\Omega))^s$, with $L_1 > 0$ independent of t.

Hence, there is a unique solution $y \in W(0,T)^s$ of the initial value problem (2.1) for every initial value $y_0 \in L^2(\Omega)^s$. Moreover, the estimate

$$\|y\|_{L^2(0,T;H^1(\Omega))^s} + \|y\|_{C([0,T];L^2(\Omega))^s} \leq C_{sol}(\|f\|_{L^2(0,T;H^1(\Omega)^*)^s} + \|y_0\|_{\Omega^s})$$

holds with a constant $C_{sol} > 0$ independent of $f, F_2, y,$ and y_0.

Proof of Theorem 2.3.2. We will adapt the method of Evans [5, Section 9.2.1] who treats one-dimensional, purely Lipschitz continuous problems with homogeneous boundary conditions. Banach's Fixed Point Theorem will be applied to the space $X := C([0,T]; L^2(\Omega))^s$, endowed with the norm $\|y\|_C^2 := \sup_{t\in[0,T]} \|y(t)\|^2_{L^2(\Omega)^s} \mathrm{e}^{-Ct}$. The constant $C > 0$ is a priori arbitrary and will be specified later on. As this modified norm is equivalent to the usual maximum norm, $(X, \|.\|_C)$ is a Banach space.

Let $y_0 \in L^2(\Omega)^s$. First, we eliminate the Lipschitz continuous reaction term from the operator equation by inserting a fixed $z \in X$. Since $F_1(z)$ belongs to $L^2(0,T;H^1(\Omega)^*)^s$, Theorem 2.2.1, applied to $F_1 = 0$, yields a unique solution $y(z) \in W(0,T)^s$ of the monotone problem

$$\begin{aligned} y' + B^s(y) + F_2(y) &= f - F_1(z) \\ y(0) &= y_0. \end{aligned} \tag{2.21}$$

Because of Theorem 1.1.2(1), the operator

$$A:\, z \mapsto y(z) \quad \text{for all } z \in X$$

maps X into itself. Obviously, y is a fixed point of A if and only if it solves the original problem (2.1).

Thanks to Banach's Fixed Point Theorem, it suffices to show the Lipschitz continuity of A with a constant in the interval $(0,1)$. To this end, we choose $z_1, z_2 \in X$ and abbreviate $y_i := A(z_i)$ for $i \in \{1,2\}$.

To establish an estimate for the difference $\delta := y_1 - y_2$, we consider the equations for $y_i(t)$ for almost every $t \in [0,T]$. Each of them can be tested with an arbitrary $v \in H^1(\Omega)^s$. Subtracting the equations from each other, we obtain due to the linearity of the first two summands on the left-hand side

$$\langle \delta'(t), v\rangle + B^s(\delta, v; t) + \langle F_2(y_1(t)) - F_2(y_2(t)), v\rangle = \langle F_1(z_2(t)) - F_1(z_1(t)), v\rangle. \tag{2.22}$$

The right-hand side f vanishes because it appears in both equations. Equation (2.22) corresponds to (2.2) in Proposition 2.2.2. The proof of the proposition's first part, applied to $Z = H^1(\Omega)$ and $z_i = y_i$, states that the equivalent of Equation (2.7)

$$\|\delta(t)\|^2_{\Omega^s} \le \mathrm{e}^{tc_1} \int_0^t \frac{2}{\kappa_{\min}} \|F_1(z_2(\sigma)) - F_1(z_1(\sigma))\|^2_{(H^1(\Omega)^*)^s} d\sigma$$

holds for all $t \in [0,T]$ with the constant $c_1 = 2\kappa_{\min} > 0$. The norm of $\delta(0)$ vanishes since $y_1(0) = y_0 = y_2(0)$. Applying the Lipschitz condition assumed for F_1, we arrive at

$$\|\delta(t)\|^2_{\Omega^s} \le \mathrm{e}^{tc_1} \int_0^t \Psi \|(z_1 - z_2)(\sigma)\|^2_{\Omega^s} d\sigma$$

with the constant $\Psi := 2L_1^2/\kappa_{\min}$. In the next step, we estimate the exponential function and the integrand after an appropriate extension. We obtain

$$\begin{aligned}\|\delta(t)\|_{\Omega^s}^2 &\le e^{Tc_1}\int_0^t \Psi\|(z_1-z_2)(\sigma)\|_{\Omega^s}^2 e^{-C\sigma}e^{C\sigma}d\sigma \le \Psi e^{Tc_1}\|z_1-z_2\|_C^2\int_0^t e^{C\sigma}d\sigma\\ &\le \frac{\Psi e^{Tc_1}}{C}\|z_1-z_2\|_C^2 e^{Ct}.\end{aligned}$$

In the last step, the remaining integral was estimated by

$$\int_0^t e^{C\sigma}d\sigma = \frac{1}{C}[e^{Ct}-1] \le \frac{1}{C}e^{Ct}.$$

Having multiplied both sides of the estimate for $\|\delta(t)\|_{\Omega^s}^2$ by e^{-Ct}, we regard its supremum. We obtain

$$\|A(z_1)-A(z_2)\|_C^2 = \sup_{t\in[0,T]}\|\delta(t)\|_{\Omega^s}^2 e^{-Ct} \le \frac{\Psi e^{Tc_1}}{C}\|z_1-z_2\|_C^2.$$

Thus, A is Lipschitz continuous with the constant

$$L_A := \sqrt{\frac{1}{C}\frac{2L_1^2}{\kappa_{\min}}e^{2T\kappa_{\min}}}.$$

The proof is valid for any $C>0$. Choosing $C > 2L_1^2\kappa_{\min}^{-1}\exp(2T\kappa_{\min})$, we obtain $L_A < 1$ due to the strict monotonicity of the square root function on $\mathbb{R}_{>0}$. Hence, the map A is a contraction on the Banach space $(X, \|.\|_C)$. Banach's Fixed Point Theorem 2.3.1 provides a unique fixed point $y \in X$ of A. Since the solutions of the initial value problem (2.1) are characterized by being a fixed point of A, the proof of existence and uniqueness is complete.

The asserted estimate of the solution y is a direct consequence of the first part of Proposition 2.2.2. By inserting an arbitrary element $v \in H^1(\Omega)^s$ as a test function into the equation for $y(t)$, we obtain

$$\langle y'(t), v\rangle + B^s(y, v; t) + \langle F_1(y(t)), v\rangle + \langle F_2(y(t)), v\rangle = \langle f(t), v\rangle$$

for almost every $t \in [0, T]$, an equivalent of Equation (2.2) with $z_1 = z = y$ and $z_2 = 0$. Proposition 2.2.2(1) yields a constant $C_{sol} > 0$ with

$$\|y\|_{L^2(0,T;H^1(\Omega))^s} + \|y\|_{C([0,T];L^2(\Omega))^s} \le C_{sol}(\|f\|_{L^2(0,T;H^1(\Omega)^*)^s} + \|y(0)\|_{\Omega^s}).$$

This is equal to the asserted estimate since $y(0) = y_0$. □

2.4 Examples

In this section, we present two reaction terms both of which are superposition operators (cf. Appell and Zabrejko [1]) associated with real functions. The first one is admitted in the regarded model class whereas the second is not.

Square root. This paragraph deals with a reaction term that fulfills the assumptions of both existence theorems of this chapter. Consider the monotone increasing and continuous real function

$$\varphi : \mathbb{R} \to \mathbb{R}, \quad \varphi(y) = \begin{cases} \sqrt{y} & \text{if } y \geq 0, \\ 0 & \text{otherwise.} \end{cases}$$

The function φ is associated with the superposition operator $d : L^2(Q_T) \to L^2(Q_T)$, defined by

$$d(y)(x,t) = \varphi(y(x,t)) \quad \text{for all } y \in L^2(Q_T) \text{ and almost all } (x,t) \in Q_T.$$

To demonstrate that d is well-defined, we observe that the function $(x,t) \mapsto \varphi(y)$ is constant and therefore measurable for all $y \in \mathbb{R}$. Furthermore, the function $y \mapsto \varphi(y)$ is continuous. Finally, the estimate $\varphi(y) \leq 1 + |y|$ is valid for all $y \in \mathbb{R}$. As a consequence, d is well-defined and continuous (cf. Appell and Zabrejko [1]). The same arguments ensure that the operators $d(t) : L^2(\Omega) \to L^2(\Omega)$, defined by $d(t)(w) = \varphi(w)$, are well-defined for every t. Finally, $W(0,T) \hookrightarrow L^2(Q_T)$. Thus, Hypothesis 1.2.1 is fulfilled.

Using Lemma 1.4.1, we can define $F : L^2(Q_T) \to L^2(0,T;H^1(\Omega)^*)$ and the family $(F(t))_t$ of operators $F(t) : L^2(\Omega) \to H^1(\Omega)^*$ on the basis of d and $(d(t))_t$, respectively. The lemma guarantees that $(F(t))_t$ generates F in the sense of (1.2). Moreover, the domains of definition $Y_2 := L^2(Q_T)$ and $\Lambda_2 := L^2(\Omega)$ fulfill (1.1).

The operators F and $F(t)$ are continuous because of the continuity of d. The continuity of F implies its demicontinuity. Furthermore, $F(t)$ is monotone because φ is monotone increasing. Since additionally $L^2(0,T;H^1(\Omega)) \hookrightarrow Y_2$, the operator F fulfills the assumptions about F_2 in both existence theorems. Thus, F is an admissible reaction term for the investigated model class. Note that F does not fulfill the assumptions about the Lipschitz continuous part F_1 because φ is not Lipschitz continuous. Thus, it makes sense to distinguish between the two types of reaction terms.

Quadratic function. This paragraph presents a monotone reaction term that does not fulfill the assumptions of the existence theorems. Consider the monotone increasing and continuous real function

$$\varphi : \mathbb{R} \to \mathbb{R}, \quad \varphi(y) = |y|y$$

and the family of operators $F(t) : H^1(\Omega) \to H^1(\Omega)^*$ defined by

$$\langle F(t)(w), z \rangle_{H^1(\Omega)^*} := \int_\Omega \varphi(w(x))z(x)dx \quad \text{for all } w, z \in H^1(\Omega), t \in [0,T].$$

To demonstrate that these operators are well-defined, let $w, z \in H^1(\Omega)$. Hölder's inequality with the exponents $3/2$ and 3 and the continuous embedding of $H^1(\Omega)$ in $L^3(\Omega)$ for $n_d \leq 3$

yield

$$\int_\Omega \varphi(w(x))z(x)dx \leq \left(\int_\Omega |w(x)|^3 dx\right)^{\frac{2}{3}} \left(\int_\Omega |z(x)|^3 dx\right)^{\frac{1}{3}} = \|w\|^2_{L^3(\Omega)} \|z\|_{L^3(\Omega)} < \infty. \quad (2.23)$$

The operators $F(t)$ are continuous and monotone but not Lipschitz continuous. Therefore, Hypothesis 2.1.1 and the existence theorems require the family $(F(t))_t$ to generate a demicontinuous operator F on a domain Y_2. The domain Y_2 has to be a superset of $L^2(0,T;H^1(\Omega))$, and the range of F has to be $L^2(0,T;H^1(\Omega)^*)$.

The smallest possible domain is $L^2(0,T;H^1(\Omega))$. However, there seems to be no continuous embedding even of this space in $L^3(Q_T)$ (or in another L^p-space with $p > 2$) comparable to the embedding of $H^1(\Omega)$ in $L^3(\Omega)$. As a consequence, finiteness of the time-dependent integral

$$\int_0^T \int_\Omega \varphi(y(x,t))v(x,t)dxdt$$

with $y, v \in L^2(0,T;H^1(\Omega))$ cannot be proved by means of Hölder's inequality.

It can be shown that the integral is finite for all $v \in L^2(0,T;H^1(\Omega))$ and $y \in W(0,T)$, i.e., the family $(F(t))_t$ generates an operator $F : W(0,T) \to L^2(0,T;H^1(\Omega)^*)$. However, the domain of definition $Y_2 = W(0,T)$ does not fulfill the assumptions of the existence theorems.

Thus, it seems that models with quadratic reaction terms belong to another class. A certain part of this class is covered by the existence result of Casas [2].

Chapter 3

Periodic solutions of models of N-DOP type

Periodic solutions are not as well investigated as transient solutions. A typical existence result for equations with monotone operators is represented by Theorem 1.1.3. Here, as well as in Shioji [24], who applies Galerkin's method to pseudo-monotone operators, a crucial assumption is the operator's coercivity. However, reaction terms belonging to mass-conserving ecosystem models normally lack this property since the conservation of mass condition (1.8) implicates that each summand added in one model equation is subtracted in another. Furthermore, most standard theorems are confined to results about existence. This is not sufficient for mass-conserving models with vanishing source terms, such as the PO_4-DOP model, since these models have the trivial function as a periodic solution.

We overcome these difficulties for an important model class to which the PO_4-DOP model belongs. The result is stated in Theorem 3.2.1. The proof is based on the standard theorem 1.1.3 and the Schauder Fixed Point Theorem, taken from Zeidler [28, Theorem 2.A]:

Theorem 3.0.1 (Schauder Fixed Point Theorem)**.** *Let M be a nonempty, closed, bounded, convex subset of a Banach space X. Suppose $A : M \to M$ is continuous and maps bounded sets into relatively compact sets (i.e., A is a compact operator). Then A has a fixed point.*

3.1 Models of N-DOP type

Models of N-DOP type generalize the PO_4-DOP model of Parekh et al. [15], presented in Chapter 4. This is already indicated by the names: The letter N is an abridged form of "nutrient" whereas PO_4 stands for the special nutrient phosphate. Like the PO_4-DOP model, a model of N-DOP type is characterized by $s = 2$ equations and a reaction term describing remineralization, i.e., a linear term multiplied with a constant ("remineralization rate"). Beyond that, models of N-DOP type can feature further reaction terms as well as nonzero source terms. In Section 4.4.2, we show that the PO_4-DOP model belongs to the class of models of N-DOP type.

As in the last chapter, we formulate a model of *N-DOP* type as an operator equation, i.e., as a variant of Equation (1.6). In the following hypothesis, we introduce the necessary spaces and operators.

Hypothesis 3.1.1. *Let $f = (f_1, f_2) \in L^2(0,T;H^1(\Omega)^*)^2$, and let Y be a Banach space in which $W(0,T)^2$ is compactly embedded. We assume that the operator $F = (F_1, F_2) : Y \to L^2(0,T;H^1(\Omega)^*)^2$ is generated by the indexed family $(F(t))_t$ of operators $F(t) : \Lambda \to (H^1(\Omega)^*)^2$ in the sense of (1.2) with $\Lambda \subseteq L^2(\Omega)^2$ fulfilling property (1.1). Furthermore, we abbreviate $B := B^1$.*

Given $\lambda > 0$, the operator $\lambda Id : L^2(0,T;H^1(\Omega)) \to L^2(0,T;H^1(\Omega)^*)$ is defined by

$$\langle \lambda Id(z), v\rangle_{L^2(0,T;H^1(\Omega)^*)} := \int_0^T \int_\Omega \lambda z(t)v(t)dxdt \quad \text{for all } z, v \in L^2(0,T;H^1(\Omega)).$$

As in the proof of Lemma 1.4.1, we can show by means of Hölder's inequality that the operator λId is well-defined. We use the slightly imprecise name Id for the embedding of $L^2(0,T;H^1(\Omega))$ in $L^2(0,T;H^1(\Omega)^*)$ to emphasize the connection between classical model equation and the corresponding operator equation. The reaction term corresponding to $\lambda Id(z)$ in the classical equation is $\lambda Id_{C^2(Q_T)}(z)$ (abbreviated by λz). In the following considerations, we will use λz to abbreviate $\lambda Id(z)$ as well.

Given Hypothesis 3.1.1, a model of *N-DOP* type corresponds to the system of operator equations

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 + F_1(y) &= f_1 \\ y_2' + B(y_2) + \lambda y_2 + F_2(y) &= f_2. \end{aligned}$$

3.2 Existence of periodic solutions

Theorem 3.2.1. *Let Hypothesis 3.1.1 be valid and let $C \in \mathbb{R}$. We assume that the reaction term $F : Y \to L^2(0,T;H^1(\Omega)^*)^2$ is continuous and that there is a constant $M_{rea} > 0$ with*

$$\max\{\|F_1(y)\|_{L^2(0,T;H^1(\Omega)^*)}, \|F_2(y)\|_{L^2(0,T;H^1(\Omega)^*)}\} \leq M_{rea} \quad \text{for all } y \in Y. \tag{3.1}$$

Suppose that the conservation of mass conditions

$$\sum_{j=1}^{2} \langle F_j(y(t)), 1\rangle_{H^1(\Omega)^*} = 0 \quad \text{and} \quad \sum_{j=1}^{2} \langle f_j(t), 1\rangle_{H^1(\Omega)^*} = 0 \tag{3.2}$$

hold for almost all $t \in [0,T]$ and all $y \in Y$. The symbol 1 stands for the element of $H^1(\Omega)$ that is equal to one almost everywhere. Hence, the periodic problem

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 + F_1(y) &= f_1 \\ y_2' + B(y_2) + \lambda y_2 + F_2(y) &= f_2 \\ y(0) &= y(T) \end{aligned} \tag{3.3}$$

has a solution $y \in W(0,T)^2$ *with* $\operatorname{mass}(y(t)) = C$ *for all* $t \in [0,T]$.

In particular, there are nontrivial periodic solutions of (3.3)*, even in case* $f_1 = f_2 = 0$.

Proof. To justify the additional statement, we regard $C \neq 0$. The theorem's main statement yields a periodic solution with the constant mass C. Since the mass is not equal to zero, the solution is nontrivial.

The proof of the main statement is divided into two steps. First, the equations are linearized and solved with the help of monotone operator theory. Afterwards, the Schauder Fixed Point Theorem yields a solution of the nonlinear problem.

Periodic solution of a linearized problem. Let $z \in Y$ be arbitrary. In this step, we show that the linear problem

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 &= f_1 - F_1(z) \\ y_2' + B(y_2) + \lambda y_2 &= f_2 - F_2(z) \\ y(0) &= y(T) \\ \operatorname{mass}(y(t)) &= C \qquad \text{for all } t \in [0,T] \end{aligned} \tag{3.4}$$

has a unique solution $y = (y_1, y_2) \in W(0,T)^2$. To this end, we apply Theorem 1.1.3 by Gajewski et al. to each equation separately. This is possible because the linearization renders the two equations in (3.4) decoupled. In particular, the problem

$$y_2' + B(y_2) + \lambda y_2 = f_2 - F_2(z), \quad y_2(0) = y_2(T)$$

can be solved independently of the first component y_1. The operator $A := B + \lambda Id : L^2(0,T;H^1(\Omega)) \to L^2(0,T;H^1(\Omega)^*)$ is linear and therefore hemicontinuous. Using Equation (1.7) in the proof of Lemma 1.4.2, we estimate

$$\begin{aligned} \langle B(y_2) + \lambda y_2, y_2 \rangle_{L^2(0,T;H^1(\Omega)^*)} &\geq \int_0^T \{\kappa_{\min} \|\nabla y_2(t)\|^2_{L^2(\Omega)^{n_d}} + \lambda \|y_2(t)\|^2_{L^2(\Omega)}\} dt \\ &\geq \min\{\kappa_{\min}, \lambda\} \|y_2\|^2_{L^2(0,T;H^1(\Omega))} \end{aligned}$$

for all $y_2 \in L^2(0,T;H^1(\Omega))$. From this it follows that A is coercive and strictly monotone. Hence, Theorem 1.1.3, applied to the evolution triple $(H^1(\Omega), L^2(\Omega), H^1(\Omega)^*)$, yields a unique periodic solution $y_2 := y_2(z) \in W(0,T)$.

Next, we consider a periodic solution y_1 of the first equation. The operator B is not coercive in the space $L^2(0,T;H^1(\Omega))$ because $B(y_1, y_1; t)$ is bounded from below only by the norm of the gradient. Therefore, we restrict B to an appropriate domain of definition, based on a new evolution triple (V, H, V^*).

We define $V := \{v \in H^1(\Omega) : \operatorname{mass}(v) = 0\}$ and $H := \overline{V}^{L^2(\Omega)}$ as the closure of V in $L^2(\Omega)$. As a sub-Hilbert space of $H^1(\Omega)$, V is reflexive and separable. Furthermore,

$\| . \|_V : V \to \mathbb{R}$, $v \mapsto \|\nabla v\|_{L^2(\Omega)^{n_d}}$ is a norm in V which is equivalent to the usual $H^1(\Omega)$-norm due to Poincaré's inequality (see e.g. Evans [5, Theorem 5.8.1]). By definition, V lies dense in H and the embedding is continuous. Therefore, (V, H, V^*) is an evolution triple. In addition, we observe

Remark 3.2.2. *Let* $v \in H$. *Then* $\operatorname{mass}(v) = 0$.

Indeed, given $v \in H$, there exists a sequence $(v_n)_n \subseteq V$ with $v_n \to v$ in $L^2(\Omega)$. Since $\operatorname{mass}(v_n) = 0$ for all n, we conclude

$$\operatorname{mass}(v) = \int_\Omega v dx = \int_\Omega (v - v_n) dx \leq \sqrt{|\Omega|} \|v - v_n\|_{L^2(\Omega)} \to 0.$$

Instead of the first equation, we solve the sum of both equations. Having obtained a periodic solution S of the sum in $W(0,T)$, the desired solution y_1 will be defined by the difference of S and y_2. By adding up both equations, we obtain the sum

$$\begin{aligned} S' + B(S) &= f_1 + f_2 - (F_1(z) + F_2(z)) \\ S(0) &= S(T). \end{aligned} \tag{3.5}$$

The condition for the mass is considered later on.

The application of Theorem 1.1.3 to (3.5) requires the coercivity of B. Therefore, we restrict the summands of the operator equation to $\tilde{B} : L^2(0,T;V) \to L^2(0,T;V^*)$ and $\tilde{f}_1 + \tilde{f}_2 - (\tilde{F}_1(z) + \tilde{F}_2(z)) \in L^2(0,T;V^*)$. The restrictions are well-defined since $L^2(0,T;V) \subseteq L^2(0,T;H^1(\Omega))$.

The restriction $\tilde{B}$ is still hemicontinuous. In addition, we estimate

$$\langle \tilde{B}(S), S \rangle_{L^2(0,T;V^*)} \geq \kappa_{\min} \int_0^T \|\nabla S(t)\|^2_{L^2(\Omega)^{n_d}} dt = \kappa_{\min} \int_0^T \|S(t)\|_V^2 dt = \kappa_{\min} \|S\|^2_{L^2(0,T;V)}$$

for all $S \in L^2(0,T;V)$ using again Equation (1.7). This estimate shows that $\tilde{B}$ is strictly monotone and coercive. Theorem 1.1.3, applied to the evolution triple (V, H, V^*), yields a unique periodic solution $S = S(z) \in W(0,T;V)$ of problem (3.5). Because of Theorem 1.1.2(1) and Remark 3.2.2, $\operatorname{mass}(S(t)) = 0$ for all $t \in [0,T]$.

Next, we prove $S \in W(0,T)$. Obviously, the initial value $S(0) \in H$ belongs to $L^2(\Omega)$. Thus, Theorem 2.2.1 provides a unique solution $S_\tau \in W(0,T)$ of the non-restricted, transient problem

$$S_\tau' + B(S_\tau) = f_1 + f_2 - (F_1(z) + F_2(z)), \quad S_\tau(0) = S(0).$$

The function $S_0 \in C([0,T]; L^2(\Omega))$, defined by $S_0(t) := S_\tau(t) - |\Omega|^{-1} \operatorname{mass}(S_\tau(t))$ for all $t \in [0,T]$, is a modification of S_τ with the constant mass 0. We investigate S_0 in the following lemma.

Lemma 3.2.3. *The modified solution has the properties* $S_0 \in L^2(0,T;V)$, $S_0' = S_\tau'$, *and* $S_0' \in L^2(0,T;H^1(\Omega)^*)$. *Furthermore,* $S_0 \in W(0,T)$ *fulfills the same equation as* S_τ.

Proof. The first property is fulfilled if $S_0 \in L^2(0,T;H^1(\Omega))$ and $\mathrm{mass}(S_0(t)) = 0$ for all t. First, the modified solution S_0 belongs to $L^2(0,T;H^1(\Omega))$ since $S_\tau \in L^2(0,T;H^1(\Omega))$ and $\mathrm{mass}(S_\tau) \in L^2(0,T)$. The latter is proved by an easy estimate using the definition of mass and Hölder's inequality. Second, let $t \in [0,T]$. We compute

$$\mathrm{mass}(S_0(t)) = \int_\Omega \left[S_\tau(t) - |\Omega|^{-1}\,\mathrm{mass}(S_\tau(t))\right] dx = \mathrm{mass}(S_\tau(t)) - |\Omega||\Omega|^{-1}\,\mathrm{mass}(S_\tau(t)) = 0.$$

Since $S_\tau' \in L^2(0,T;H^1(\Omega)^*)$, the third assertion follows from the second. Because of the definition of S_0, the second assertion is equivalent to the weak differentiability of the map $\mathrm{mass}(S_\tau) : [0,T] \to \mathbb{R}$ with the derivative $\mathrm{mass}(S_\tau)' = 0$.

The function S_τ solves the operator equation investigated in Theorem 1.5.3 with $s = 1$, $\tilde{F} = 0$ and $\tilde{f} = f_1 + f_2 - (F_1(z) + F_2(z))$. Since $\langle \tilde{f}(t), 1\rangle_{H^1(\Omega)^*} = 0$ for almost all $t \in [0,T]$ by assumption, the theorem yields $\frac{\mathrm{d}}{\mathrm{dt}}\,\mathrm{mass}(S_\tau(t)) = 0$ for almost all t. This proves the second claim of the lemma.

Finally, the third assertion and $S_0 \in L^2(0,T;H^1(\Omega))$, proved in connection with the first assertion, imply $S_0 \in W(0,T)$. The second assertion, the definition of S_0, Lemma 1.4.2(4), applied to $c(t) = -|\Omega|^{-1}\,\mathrm{mass}(S_\tau(t))$, and the equation for S_τ yield

$$S_0' + B(S_0) = S_\tau' + B(S_\tau - |\Omega|^{-1}\,\mathrm{mass}(S_\tau)) = S_\tau' + B(S_\tau) = f_1 + f_2 - (F_1(z) + F_2(z)).$$

Therefore, the forth assertion of the lemma holds true as well. □

In particular, the lemma shows that S_0 belongs to $W(0,T)$. Below, we will prove that S_0 equals S. These properties imply the desired statement $S \in W(0,T)$.

To prove $S_0 = S$, we show that $\delta := S - S_0$ vanishes. The difference δ belongs to $L^2(0,T;V)$ and therefore also to $L^2(0,T;H^1(\Omega))$. Thus, $\delta(t)$ can be inserted into the operators of the equations for both $S_0(t)$ and $S(t)$. The difference of both equations equals $\langle \delta'(t), \delta(t)\rangle_{V^*} + B(\delta,\delta;t) = 0$ for almost every t. Theorem 1.1.2(2) and Equation (1.7) in the proof of Lemma 1.4.2 yield

$$\frac{d}{dt}\|\delta(t)\|_H^2 \leq -2\kappa_{\min}\|\nabla\delta(t)\|_{L^2(\Omega)^{n_d}}^2 \leq 0 \quad \text{for almost all } t.$$

Consequentially, we obtain using Gronwall's lemma

$$\begin{aligned}\|\delta(t)\|_H^2 \leq \exp(0)\|\delta(0)\|_H^2 &= \|S(0) - [S_\tau(0) - |\Omega|^{-1}\,\mathrm{mass}(S_\tau(0))]\|_H^2 \\ &= \|S(0) - S(0) + |\Omega|^{-1}\,\mathrm{mass}(S(0))\|_H^2 = 0\end{aligned}$$

for every $t \in [0,T]$. The first equality sign holds because of the definition of S_0, and the second is due to $S_\tau(0) = S(0)$. In the last step, we use $\mathrm{mass}(S(0)) = 0$. We conclude $S(t) = S_0(t)$ for all $t \in [0,T]$, i.e., $S = S_0$.

In summary, we have verified that $S(z) := S \in W(0,T) \cap L^2(0,T;V)$ solves problem (3.5) and has the constant mass zero. Thus, we are able to define the candidate for a solution of the first equation

$$y_1 := S - y_2 + C|\Omega|^{-1} \in W(0,T).$$

The constant summand $C|\Omega|^{-1}$ serves to adjust the mass. The candidate y_1 is periodic since the same is true for S, y_2, and the constant $C|\Omega|^{-1}$. Moreover, it solves the first equation of problem (3.4). Indeed, if we insert the definition of y_1 into B and the temporal derivative on the left-hand side of this equation, the constant $C|\Omega|^{-1}$ vanishes. Then, we rearrange the remaining summands and use the equations for S and y_2. We obtain

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 &= (S - y_2 + C|\Omega|^{-1})' + B(S - y_2 + C|\Omega|^{-1}) - \lambda y_2 \\ &= S' + B(S) - (y_2' + B(y_2) + \lambda y_2) = f_1 + f_2 - (F_1(z) + F_2(z)) - (f_2 - F_2(z)) \\ &= f_1 - F_1(z). \end{aligned}$$

Finally, the mass of $y := (y_1, y_2) \in W(0,T)^2$ is equal to

$$\text{mass}(y(t)) = \int_\Omega (y_1(t) + y_2(t))dx = \int_\Omega (S(t) + C|\Omega|^{-1})dx = C \quad \text{for all } t \in [0,T]$$

since $\text{mass}(S(t)) = 0$ for all t. Thus, y solves problem (3.4). The uniqueness of y is an immediate consequence of the previous results. Given two solutions $y, \tilde{y}$ of (3.4), the existence theorem 1.1.3 yields $y_2 = \tilde{y}_2$. The difference $\delta := y_1 - \tilde{y}_1$ is a periodic solution of the equation $\delta' + B(\delta) = 0$. Since both y and $\tilde{y}$ have the constant mass C and $y_2 = \tilde{y}_2$, we obtain

$$\text{mass}(\delta(t)) = \text{mass}(y_1(t)) - \text{mass}(\tilde{y}_1(t)) = C - \text{mass}(y_2(t)) - (C - \text{mass}(\tilde{y}_2(t))) = 0$$

for all $t \in [0,T]$, i.e., δ belongs to $L^2(0,T;V)$. In connection with the difference $S - S_0$, we have shown that the equation $\delta' + B(\delta) = 0$ is uniquely solvable in $L^2(0,T;V)$. Obviously, the constant zero function is this solution. Thus, $\delta = 0$, and the solution of (3.4) is unique.

Result 3.2.4. *Given a fixed $z \in Y$, the pair $y(z) := (y_1, y_2) \in W(0,T)^2$ is a unique solution of the linearized problem* (3.4).

Periodic solution of the nonlinear problem. The solution $y(z)$ of problem (3.4) belongs to Y since $W(0,T)^2$ is a subset of Y by assumption. For this reason, the operator

$$A : Y \to Y, \quad z \mapsto y(z)$$

is well-defined. Obviously, y is a fixed point of A if and only if it is a solution of the original problem (3.3) with $\text{mass}(y(t)) = C$ for all $t \in [0,T]$.

We will prove the existence of a fixed point of A by means of the Schauder Fixed Point Theorem. For this, we need an estimate of periodic solutions.

Lemma 3.2.5. *Let $W \in \{V, H^1(\Omega)\}$, $R \in L^2(0,T;H^1(\Omega)^*)$, and $\gamma \geq 0$. Suppose that $w \in W(0,T;W)$ is a periodic solution of $w' + B(w) + \gamma w = R$.*

If either $\gamma > 0$ or $W = V$, there is a constant K, only depending on $\gamma, \kappa_{\min}$, and the Poincaré constant, such that

$$\|w\|_{L^2(0,T;H^1(\Omega))} \leq K\|R\|_{L^2(0,T;H^1(\Omega)^*)}.$$

Proof. Applying the operator equation to $w \in W(0,T;W)$ itself, we obtain

$$\langle w'(t), w(t)\rangle_{W^*} + B(w,w;t) + \gamma\|w(t)\|^2_{L^2(\Omega)} = \langle R(t), w(t)\rangle_{H^1(\Omega)^*} \quad \text{for almost every } t.$$

We transform the first two summands using Theorem 1.1.2(2) and Equation (1.7) and estimate the right-hand side by means of Cauchy's inequality with ε (see e.g. Evans [5, Appendix B.2]). We conclude

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2(\Omega)} + \kappa_{\min}\|\nabla w(t)\|^2_{L^2(\Omega)^{n_d}} + \gamma\|w(t)\|^2_{L^2(\Omega)} \leq \frac{1}{4\varepsilon}\|R(t)\|^2_{H^1(\Omega)^*} + \varepsilon\|w(t)\|^2_{H^1(\Omega)} \tag{3.6}$$

for every $\varepsilon > 0$. Since H and $L^2(\Omega)$ have the same norm, the first summand is the same for both possible spaces W. In case $\gamma > 0$, Equation (3.6) with $\varepsilon_1 := \min\{\kappa_{\min}, \gamma\}/2 > 0$ can be transformed into

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2(\Omega)} + \frac{1}{2}\min\{\kappa_{\min},\gamma\}\|w(t)\|^2_{H^1(\Omega)} \leq \frac{1}{2\min\{\kappa_{\min},\gamma\}}\|R(t)\|^2_{H^1(\Omega)^*}.$$

In case $\gamma = 0$, we assume $W = V$. Since the norm of the gradient is equivalent to the usual $H^1(\Omega)$-norm on V, there is a constant $k > 0$, depending only on the Poincaré constant, with $k\|w(t)\|_{H^1(\Omega)} \leq \|\nabla w(t)\|_{L^2(\Omega)^{n_d}}$. We infer from (3.6) with $\varepsilon_2 := k^2\kappa_{\min}/2$

$$\frac{1}{2}\frac{d}{dt}\|w(t)\|^2_{L^2(\Omega)} + \frac{1}{2}k^2\kappa_{\min}\|w(t)\|^2_{H^1(\Omega)} \leq \frac{1}{2k^2\kappa_{\min}}\|R(t)\|^2_{H^1(\Omega)^*}.$$

Thus, a comparable inequality holds in both cases. The first summand vanishes after an integration over $[0,T]$ because of Theorem 1.1.2(3) and the periodicity of w. As a consequence, the desired estimate holds with $K := \max\{1/k^2\kappa_{\min}, 1/\min\{\kappa_{\min},\gamma\}\}$. □

In the remainder of this proof, we demonstrate that the operator A fulfills the assumptions of the Schauder Fixed Point Theorem. To define the domain of definition M of A, we show that the range of A is bounded in $W(0,T)^2$, i.e., that the norm of $A(z)$ is bounded independently of $z \in Y$.

Let $z \in Y$. As to the second component of $y := A(z)$, Lemma 3.2.5, applied to $w := y_2$, $\gamma := \lambda > 0$ and $R := f_2 - F_2(z)$, yields $\|y_2\|_{L^2(0,T;H^1(\Omega))} \leq K_1\|f_2 - F_2(z)\|_{L^2(0,T;H^1(\Omega)^*)}$. Since the first component is defined by $y_1 = S - y_2 + |\Omega|^{-1}C$, the boundedness of S implies the boundedness of y_1. The lemma, applied to $w := S$, $\gamma := 0$, $W := V$ and $R := f_1 + f_2 - (F_1(z) + F_2(z))$, yields $\|S\|_{L^2(0,T;H^1(\Omega))} \leq K_2\|f_1 + f_2 - (F_1(z) + F_2(z))\|_{L^2(0,T;H^1(\Omega)^*)}$.

Because of the boundedness condition (3.1), we obtain $\|y_2\|_{L^2(0,T;H^1(\Omega))} \leq C_1$ and

$$\|y_1\|_{L^2(0,T;H^1(\Omega))} \leq \|S\|_{L^2(0,T;H^1(\Omega))} + \||\Omega|^{-1}C\|_{L^2(0,T;H^1(\Omega))} + \|y_2\|_{L^2(0,T;H^1(\Omega))} \leq C_2$$

with C_1 and C_2 depending on M_{rea} as well as on K_j and f_j for each $j \in \{1,2\}$ but not on z.

Furthermore, the derivative $y' = (y_1', y_2')$ can be estimated according to the additional statement of Proposition 2.2.2(2) because the reaction term $(-\lambda Id, \lambda Id)$ is homogeneous and Lipschitz continuous. The proposition provides a constant $\tilde{C} > 0$ with

$$\|y'\|_{L^2(0,T;H^1(\Omega)^*)^2} \leq \tilde{C}\left(\|f - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2} + \|y\|_{L^2(0,T;H^1(\Omega))^2}\right).$$

According to the previous results and the assumption (3.1), the right-hand side of this estimate is bounded from above by a constant $C_3 > 0$ which is independent of z.

Result 3.2.6. *Given $z \in Y$, the $W(0,T)^2$-norm of $A(z)$ is bounded independently of z by a constant C_4.*

Because of the compact and thus continuous embedding of $W(0,T)^2$ in Y, there is a constant $c_W > 0$ with $\|w\|_Y \leq c_W \|w\|_{W(0,T)^2}$ for all $w \in W(0,T)^2$. We define the set

$$M := \{y \in Y : \|y\|_Y \leq c_W C_4\}.$$

The set M is an appropriate domain of definition for A if the range $A(M)$ lies in M. To prove this, let $z \in M$. Result 3.2.6 and the continuous embedding yield

$$\|A(z)\|_Y \leq c_W \|A(z)\|_{W(0,T)^2} \leq c_W C_4. \tag{3.7}$$

Thus, $A(M) \subseteq M$, and the operator $A : M \to M$ is well-defined.

Since M is a closed ball in Y with a positive radius, it is nonempty, closed, bounded, and convex. In addition, we prove the compactness of A, i.e., first, that A is continuous and, second, that A maps bounded sets into relatively compact sets. To prove the second property, let $\tilde{M} \subseteq M$ be a bounded set. According to Result 3.2.6, $A(\tilde{M})$ lies in the closed ball with radius C_4 in $W(0,T)^2$. Being bounded, this ball is relatively compact in Y because, by assumption, the identity map from $W(0,T)^2$ to Y is compact. As a subset of a relatively compact set, $A(\tilde{M})$ itself is relatively compact.

To prove the continuity of A, let $z, \tilde{z} \in Y$. The difference $\delta := A(z) - A(\tilde{z})$ is a periodic solution of

$$\begin{aligned} \delta_1' + B(\delta_1) - \lambda\delta_2 &= F_1(\tilde{z}) - F_1(z) \\ \delta_2' + B(\delta_2) + \lambda\delta_2 &= F_2(\tilde{z}) - F_2(z). \end{aligned}$$

Lemma 3.2.5, applied to $w := \delta_2$, $\gamma := \lambda$, and $R := F_2(\tilde{z}) - F_2(z)$, yields the estimate

$$\|A(z)_2 - A(\tilde{z})_2\|_{L^2(0,T;H^1(\Omega))} \leq K_3 \|F_2(\tilde{z}) - F_2(z)\|_{L^2(0,T;H^1(\Omega)^*)}$$

for the second component of δ with a constant $K_3 > 0$. Because of

$$\delta_1 = S(z) + |\Omega|^{-1}C - A(z)_2 - (S(\tilde{z}) + |\Omega|^{-1}C - A(\tilde{z})_2) = S(z) - S(\tilde{z}) - \delta_2,$$

it suffices to estimate the difference $S(z) - S(\tilde{z}) \in L^2(0,T;V)$, the periodic solution of

$$(S(z) - S(\tilde{z}))' + B(S(z) - S(\tilde{z})) = F_1(\tilde{z}) + F_2(\tilde{z}) - (F_1(z) + F_2(z)),$$

instead of δ_1. Lemma 3.2.5, applied to $w := S(z) - S(\tilde{z})$, $\gamma := 0$, $W := V$, and $R := F_1(\tilde{z}) - F_1(z) + F_2(\tilde{z}) - F_2(z)$, and the triangle inequality yield

$$\|S(z) - S(\tilde{z})\|_{L^2(0,T;H^1(\Omega))} \leq K_4 \big(\|F_1(\tilde{z}) - F_1(z)\|_{L^2(0,T;H^1(\Omega)^*)} + \|F_2(\tilde{z}) - F_2(z)\|_{L^2(0,T;H^1(\Omega)^*)}\big)$$

with a constant $K_4 > 0$. Combining the previous results, we obtain a constant $K_5 > 0$ with

$$\|A(z) - A(\tilde{z})\|_{L^2(0,T;H^1(\Omega))^2} \leq K_5 \|F(\tilde{z}) - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2}.$$

As above, δ' can be estimated by means of the additional statement of Proposition 2.2.2(2). Combining all results, we obtain a constant $K_6 > 0$ with

$$\|A(z) - A(\tilde{z})\|_{W(0,T)^2} \leq K_6 \|F(\tilde{z}) - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2} \quad \text{for all } z, \tilde{z} \in Y.$$

Let $\varepsilon > 0$. The continuity of $F : Y \to L^2(0,T;H^1(\Omega)^*)^2$ implies that there exists $\zeta > 0$ with

$$\|F(\tilde{z}) - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2} < \frac{\varepsilon}{c_W K_6} \quad \text{provided that } \|\tilde{z} - z\|_Y < \zeta.$$

This estimate, combined with the continuous embedding of $W(0,T)^2$ in Y and the estimate of $A(z) - A(\tilde{z})$ in $W(0,T)^2$, yields

$$\|A(z) - A(\tilde{z})\|_Y \leq c_W \|A(z) - A(\tilde{z})\|_{W(0,T)^2} \leq c_W K_6 \|F(\tilde{z}) - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2} < \varepsilon$$

provided that $\|\tilde{z} - z\|_Y < \zeta$. Thus, A is continuous.

Since A fulfills all assumptions of the Schauder Fixed Point Theorem, we obtain a fixed point $y \in M$ of A. The definition of A ensures that y belongs to $W(0,T)^2$, solves

$$\begin{aligned} y_1' + B(y_1) - \lambda y_2 - F_1(y) &= f_1 \\ y_2' + B(y_2) + \lambda y_2 - F_2(y) &= f_2 \\ y(0) &= y(T), \end{aligned}$$

and fulfills $\mathrm{mass}(y(t)) = C$ for all $t \in [0, T]$. □

3.3 Stationary solutions

This section is concerned with stationary solutions of models of *N-DOP* type. Since stationary and periodic solutions are related, the existence of both types of solutions can be proved with the same strategy (linearization and fixed point argument). In the stationary case, the linearized equation is solved by means of the Browder-Minty theorem. We cite this theorem from Zeidler [29, Theorem 26.A]).

Theorem 3.3.1 (Browder-Minty). *Let $A : X \to X^*$ be a monotone, coercive, and hemicontinuous operator on the real, separable, reflexive Banach space X. Then, for each $b \in X^*$ the operator equation $A(u) = b$ has a solution in X. If the operator A is strictly monotone, then the equation is uniquely solvable.*

The assumptions about the operator A (monotone, coercive, hemicontinuous) reveal the relationship between the theorems of Browder-Minty and Gajewski et al. (Theorem 1.1.3).

Let Hypothesis 3.1.1 be valid with the additional assumption that F and f are constant with respect to time. We formulate the stationary problem as in Section 1.6. The linear operator $B_{stat} : H^1(\Omega) \to H^1(\Omega)^*$ is defined by $B_{stat} := B^1_{stat}$. The additional assumption permits the restriction of F and f to time-independent domains of definition. We denote the restrictions by $F_{stat} : \Lambda \to (H^1(\Omega)^*)^2$ and $f_{stat} \in (H^1(\Omega)^*)^2$. Similarly, λId can be regarded as an operator from $H^1(\Omega)$ to $H^1(\Omega)^*$.

A stationary solution y belongs to $H^1(\Omega)^2 \cap \Lambda$ and satisfies

$$\begin{aligned} B_{stat}(y_1) - \lambda y_2 + F_{stat,1}(y) &= f_{stat,1} \\ B_{stat}(y_2) + \lambda y_2 + F_{stat,2}(y) &= f_{stat,2}. \end{aligned} \tag{3.8}$$

Theorem 3.3.2. *Beside Hypothesis 3.1.1, we assume that F and f are constant and that $H^1(\Omega)^2$ is compactly embedded in Λ. Let B_{stat}, F_{stat}, and f_{stat} be defined as above and let $C \in \mathbb{R}$. We assume that F_{stat} is continuous and that there is a constant $M_{stat} > 0$ with*

$$\max\{\|F_{stat,1}(y)\|_{H^1(\Omega)^*}, \|F_{stat,2}(y)\|_{H^1(\Omega)^*}\} \le M_{stat} \quad \text{for all } y \in \Lambda.$$

Suppose that the conservation of mass conditions

$$\sum_{j=1}^{2} \langle F_{stat,j}(y), 1\rangle_{H^1(\Omega)^*} = 0 \quad \text{and} \quad \sum_{j=1}^{2} \langle f_{stat,j}, 1\rangle_{H^1(\Omega)^*} = 0$$

hold for all $y \in \Lambda$. The symbol 1 stands again for the element of $H^1(\Omega)$ that is equal to one almost everywhere. Hence, the stationary equation (3.8) has a solution $y \in H^1(\Omega)^2$ with $\mathrm{mass}(y) = C$.

Even if $f_{stat,1} = f_{stat,2} = 0$, there are nontrivial solutions of (3.8).

Proof. We proceed as in the proof of Theorem 3.2.1 and concentrate on explaining the differences. In the first step, we choose an arbitrary element $z \in \Lambda$ and solve the problem

$$B_{stat}(y_1) - \lambda y_2 = f_{stat,1} - F_{stat,1}(z)$$
$$B_{stat}(y_2) + \lambda y_2 = f_{stat,2} - F_{stat,2}(z).$$

The Browder-Minty Theorem 3.3.1 yields the unique solutions $y_2(z) \in H^1(\Omega)$ of the second equation and $S(z) \in V$ of the sum equation $B_{stat}(S) = \sum_{j=1}^{2} (f_{stat,j} - F_{stat,j}(z))$ restricted to V^*. Coercivity and strict monotonicity of B_{stat} are proved as in the periodic case.

The solution $S := S(z) \in H^1(\Omega)$ fulfills the sum equation in $H^1(\Omega)^*$ instead of V^*. This is an immediate consequence of the representation $w = w_0 + |\Omega|^{-1} \operatorname{mass}(w)$ with $w_0 := w - |\Omega|^{-1} \operatorname{mass}(w) \in V$ for every test function $w \in H^1(\Omega)$. Since $w_0 \in V$ is a proper test function for the sum equation in V^*, we obtain

$$\begin{aligned}\langle B_{stat}(S), w\rangle_{H^1(\Omega)^*} &= \langle B_{stat}(S), w_0\rangle_{V^*} + \langle B_{stat}(S), |\Omega|^{-1} \operatorname{mass}(w)\rangle_{H^1(\Omega)^*} \\ &= \sum_{j=1}^{2} \langle f_{stat,j} - F_{stat,j}(z), w_0\rangle_{V^*} = \sum_{j=1}^{2} \langle f_{stat,j} - F_{stat,j}(z), w\rangle_{H^1(\Omega)^*}.\end{aligned}$$

The expression $\langle B_{stat}(S), |\Omega|^{-1} \operatorname{mass}(w)\rangle_{H^1(\Omega)^*}$ vanishes because of Lemma 1.4.2(3). In the last step, we use $\sum_{j=1}^{2} \langle f_{stat,j} - F_{stat,j}(z), |\Omega|^{-1} \operatorname{mass}(w)\rangle_{H^1(\Omega)^*} = 0$, a conclusion from the conservation of mass condition. Thus, S is a solution of the sum equation in $H^1(\Omega)^*$.

As in the periodic case, we conclude that $y_1(z) := S(z) - y_2(z) + |\Omega|^{-1}C$ solves the first equation and that $y(z) := (y_1(z), y_2(z)) \in H^1(\Omega)^2 \subseteq \Lambda$ is a unique solution of the linearized problem. As a consequence, the operator $A_{stat} : \Lambda \to \Lambda, z \mapsto y(z)$ is well-defined.

The fixed point argument in the second step can be transferred almost directly from the periodic case. The proof of Lemma 3.2.5, adapted to the time-independent case, shows that the $H^1(\Omega)$-norms of $y_2(z)$ and $S(z)$ are bounded by the norms of the corresponding right-hand sides. These estimates, combined with the boundedness condition for F_{stat}, yield that the range $A_{stat}(\Lambda)$ is bounded in $H^1(\Omega)^2$. The range is bounded in Λ as well since $H^1(\Omega)^2$ is continuously embedded in Λ. As a consequence, A_{stat} maps a closed ball $M \subseteq \Lambda$, bounded in Λ as well as in $H^1(\Omega)^2$, into itself.

The range $A_{stat}(\tilde{M})$ of a bounded subset $\tilde{M}$ of M is also a subset of M and thus bounded in $H^1(\Omega)^2$. This property, combined with the compact embedding of $H^1(\Omega)^2$ in Λ, yields that $A_{stat}(\tilde{M})$ is relatively compact in Λ. As in the periodic case, the continuity assumed for F_{stat} implies the continuity of A_{stat}. Thus, the Schauder Fixed Point Theorem yields a fixed point of A_{stat} which is a solution of the nonlinear stationary problem and has the mass C. □

Remark 3.3.3. *In the proof of Theorem 3.3.2, the Browder-Minty Theorem is applied to linear equations only. Therefore, it is possible to use the Lax-Milgram Theorem (cf. Evans [5, Section 6.2.1]) instead. However, we choose the more abstract result by Browder and Minty* *to emphasize the analogy to the periodic case. Furthermore, the Browder-Minty Theorem applies to operator equations. To use the Lax-Milgram Theorem, we would have to regard* B_{stat} *as a bilinear form, i.e., return to a weak formulation in the sense of Equation* (1.4).

Chapter 4

The PO_4-DOP(-Fe) model

The PO_4-DOP model of Parekh et al. [15] is a well-known example for a marine ecosystem model of N-DOP type. Because of its relatively low complexity, this model is valuable for testing purposes. In the hierarchy of models by Kriest et al. [10], it is the second simplest. The PO_4-DOP model describes the marine phosphorus cycle by means of the concentrations of phosphate (PO_4) and dissolved organic phosphorus (DOP). It is introduced as a part of the PO_4-DOP-Fe model, representing the relation between the iron concentration and the phosphorus cycle. The extended model consists of three equations characterizing the concentrations of PO_4, DOP, and iron (Fe). The underlying ocean domain is assumed to be three-dimensional, i.e., $n_d = 3$.

In Section 4.4, we investigate the PO_4-DOP-Fe model regarding transient and the PO_4-DOP model regarding transient, periodic and stationary solutions. Prior to that, we introduce the models according to Parekh et al. [15]. We enhance the model's original formulation by important information required for the mathematical analysis, such as the definition of the domain Ω, the underlying function spaces, and boundary conditions.

4.1 The domain

The modeled ecosystem is located in a three-dimensional bounded domain $\Omega \subseteq \mathbb{R}^3$. The domain is determined by the open, bounded water surface $\Omega' \subseteq \mathbb{R}^2$ and the depth $h(x') > 0$ at every surface point $x' \in \Omega'$. The function $h : \Omega' \to \mathbb{R}_+$ is Lipschitz continuous and bounded by the total depth of the ocean $h_{max} > 0$. Thus, $\Omega = \{(x', x_3) : x' \in \Omega', x_3 \in (0, h(x'))\}$. The boundary $\Gamma := \partial\Omega$ is the union of the surface $\Gamma' := \overline{\Omega'} \times \{0\}$ and the boundary inside the water.

The domain is separated into two layers, the euphotic, light-flooded zone Ω_1 below the surface and the subjacent aphotic zone Ω_2 without incidence of light. The maximum depth of the euphotic zone is denoted by $\bar{h}_e$. The actual depth of the euphotic zone beneath a surface point $x' \in \Omega'$ is defined by $h_e(x') := \min\{\bar{h}_e, h(x')\}$. We split the surface into the part $\Omega'_2 := \{x' \in \Omega' : h(x') > \bar{h}_e\}$ above the aphotic zone and the rest $\Omega'_1 := \Omega' \setminus \Omega'_2$. Using these definitions, we divide Ω and Γ into the sets

- the euphotic zone $\Omega_1 := \{(x', x_3) : x' \in \Omega', x_3 \in (0, h_e(x'))\}$,
- the aphotic zone $\Omega_2 := \{(x', x_3) : x' \in \Omega'_2, x_3 \in (\bar{h}_e, h(x'))\}$,
- the euphotic boundary $\Gamma_1 := \{(x', h(x')) : x' \in \overline{\Omega'_1}\}$,
- the aphotic boundary $\Gamma_2 := \{(x', h(x')) : x' \in \Omega'_2\}$,
- the surface $\Gamma' := \overline{\Omega'} \times \{0\}$.

4.2 The PO_4-DOP model

To be consistent with the notation of the previous chapters, we abbreviate the two model variables by $y_1 := PO_4$ and $y_2 := DOP$, assembled in the vector $y = (y_1, y_2)$. The model in classical form is the equivalent of the system (1.3) with two equations

$$\left.\begin{array}{rcll} \partial_t y_j + \mathbf{v} \cdot \nabla y_j - \operatorname{div}(\kappa \nabla y_j) + d_j(y) & = & q_{Q_T j} & \text{in } Q_T \\ \nabla y_j \cdot (\kappa \eta) + b_j(y) & = & q_{\Sigma j} & \text{in } \Sigma \end{array}\right\} \quad \text{for all } j \in \{1, 2\}.$$

The PO_4-DOP model describes a cycle. Therefore, the right-hand sides are zero, i.e., $q_{Q_T} := 0$ and $q_\Sigma := 0$.

We introduce the reaction term d in Section 4.2.2 and derive the boundary term b in Section 4.2.3. The most important reaction, the uptake of phosphate in the context of photosynthesis, is described by Michaelis-Menten kinetics. According to this theory, the reaction rate approaches a maximum at high concentrations of the influencing factors (here nutrients and light). Mathematically, this limitation is expressed by saturation functions. First of all, we introduce this kind of function.

4.2.1 Saturation functions

Let $K > 0$. A saturation function with half saturation constant K is defined by

$$f_K : \mathbb{R} \to \mathbb{R}, \quad f_K(x) := \frac{x}{|x| + K}.$$

The constant indicates the concentration x at which the reaction rate f_K is half of the maximum (here 1).

Variants of the function f_K appear in many ecosystem models, such as the PO_4-DOP model, the $NPZD$ model of Oschlies and Garçon [14] (see also Rückelt et al. [20]), or the model of McKinley et al. [12]. In these examples, the modulus in the denominator is missing since concentrations are considered to be nonnegative. However, in the context of the mathematical analysis, we cannot assume without further investigation that the solutions of ecosystem model equations are nonnegative. Beyond that, the modulus ensures that reaction terms based on f_K are defined on a whole Banach space Y which is required by Hypothesis 1.2.1.

In the next lemma, we state some essential properties of f_K.

Lemma 4.2.1. *The real function f_K is Lipschitz continuous with the constant $1/K$, and $|f_K|$ is bounded by 1. Furthermore, f_K is once, but not twice differentiable.*

Proof. If $x \neq 0$, we use $|x| + K \geq |x|$ to conclude

$$|f_K(x)| = \left| \frac{x}{|x| + K} \right| \leq \frac{|x|}{|x|} = 1.$$

Since $f_K(0) = 0$, the function $|f_K|$ is bounded by 1. Next, we show that f_K is once differentiable. The modulus $|x|$ in the denominator forces us to regard the differentiability at $x = 0$ separately. Since the occurring limits exist, we conclude

$$f'_K(0+) = \lim_{t \downarrow 0} \frac{f_K(0+t) - f_K(0)}{t} = \lim_{t \downarrow 0} \frac{1}{t} \frac{t}{t+K} = \lim_{t \downarrow 0} \frac{1}{t+K} = \frac{1}{K} = \frac{K}{(|0| + K)^2},$$
$$f'_K(0-) = \lim_{t \uparrow 0} \frac{f_K(0+t) - f_K(0)}{t} = \lim_{t \uparrow 0} \frac{1}{t} \frac{t}{-t+K} = \lim_{t \uparrow 0} \frac{1}{-t+K} = \frac{1}{K} = \frac{K}{(|0| + K)^2}.$$

Since the one-sided limits are equal, f_K is differentiable at $x = 0$. The differentiability at $x \in \mathbb{R} \setminus \{0\}$ follows from the fact that f_K is a composition of differentiable functions. The derivative can be determined via the quotient rule as

$$f'_K(x) = \frac{d}{dx} \frac{x}{x+K} = \frac{x + K - x}{(x+K)^2} = \frac{K}{(x+K)^2} = \frac{K}{(|x| + K)^2} \qquad \text{for } x > 0,$$
$$f'_K(x) = \frac{d}{dx} \frac{x}{-x+K} = \frac{-x + K + x}{(-x+K)^2} = \frac{K}{(-x+K)^2} = \frac{K}{(|x| + K)^2} \qquad \text{for } x < 0.$$

Thus, f_K is once differentiable.

We prove the Lipschitz continuity by virtue of the mean value theorem. The estimate $|x| + K \geq K$ implies $|f'_K(x)| = K/(|x| + K)^2 \leq 1/K$. The mean value theorem yields

$$|f_K(x) - f_K(y)| \leq \sup_{\xi \in \mathbb{R}} |f'_K(\xi)||x - y| \leq \frac{1}{K}|x - y| \quad \text{for all } x, y \in \mathbb{R},$$

the Lipschitz continuity of f_K with the constant $1/K$.

Finally, we demonstrate that f'_K is not differentiable at $x = 0$. To this end, we compute the difference quotient

$$\frac{f'_K(0+t) - f'_K(0)}{t} = \frac{1}{t} \left(\frac{K}{(|t| + K)^2} - \frac{1}{K} \right) = \frac{K^2 - (|t| + K)^2}{t(|t| + K)^2 K} = \frac{-t - \operatorname{sgn}(t) 2K}{(|t| + K)^2 K}$$

for all $t \in \mathbb{R} \setminus \{0\}$. This result directly yields that the one-sided limits $f''_K(0+) = -2/K^2$ and $f''_K(0-) = 2/K^2$ are not equal. Thus, f_K is not twice differentiable. □

4.2.2 Reaction terms in Ω

A typical biogeochemical process considered in models of *N-DOP* type is the remineralization of organic material (cf. Section 3.1). The PO_4-*DOP* model includes this reaction as well. Remineralization is modeled as a linear transformation of y_2 into y_1 with a remineralization rate $\lambda > 0$. Being independent of light, this process occurs in the whole domain Ω.

The remaining processes are influenced by light and thus differ depending on the layer. The most important process is the consumption (or uptake) of phosphate in the context of photosynthesis in the euphotic zone Ω_1. The maximum uptake rate $\alpha > 0$ is limited by the light intensity and the available concentrations of phosphate and iron. Using saturation functions to model these limitations, Parekh et al. [15] express the uptake at $(x, t) \in \Omega_1 \times [0, T]$ by

$$G(y_1, y_3, x, t) := \alpha \frac{y_1(x,t)}{|y_1(x,t)| + K_P} \frac{I(x', t)\mathrm{e}^{-x_3 K_W}}{|I(x', t)\mathrm{e}^{-x_3 K_W}| + K_I} \frac{y_3(x,t)}{|y_3(x,t)| + K_F}. \tag{4.1}$$

In anticipation of the PO_4-*DOP-Fe* model, we refer to the concentration of iron as y_3 although it is not variable in the PO_4-*DOP* model. The positive half saturation constants for phosphate, insolation, and iron are called K_P, K_I, and K_F, respectively. Insolation at the water surface is expressed by a nonnegative, bounded function $I : \Omega' \times [0, T] \to \mathbb{R}_+$ which is continuous with respect to t. Beneath the surface, the light intensity exponentially decreases with depth. The decrease is controlled by the attenuation coefficient for water $K_W > 0$ (cf. Rückelt et al. [20], Prieß et al. [17]).

Parekh et al. [16] formulate the uptake slightly differently to comply with Liebig's law of the minimum. In their version, the product of the saturation functions for y_1 and y_3 is replaced by the minimum. However, this alternative function is not differentiable and thus incompatible with the hypothesis of Chapter 5 about parameter identification. Therefore, we use the original formulation of Parekh et al. [15].

In the context of the PO_4-*DOP* model, the iron concentration y_3 is assumed to be constant and nonnegative. As a consequence, the fraction $y_3(x,t)/(|y_3(x,t)| + K_F)$ is constant and nonnegative as well. If α is redefined as the product of the original α and the constant fraction, the fraction and y_3 leave the definition of G.

In the remainder of this section, we formulate the PO_4-*DOP* model's reaction terms in compliance with Hypothesis 1.2.1, i.e., as operators on the space $Y := L^2(Q_T)^2$ with associated indexed families on the domain of definition $\Lambda := L^2(\Omega)^2$. The spaces Y and Λ are in accordance with Hypothesis 1.2.1 since the lemma of Aubin and Lions (Růžička [19, Lemma 3.74]) guarantees that the space $W(0, T)$ is compactly and therefore continuously embedded in $L^2(Q_T)$ in case $n_d = 3$. Furthermore, Λ obviously fulfills the condition (1.1).

We start with the definition of the reaction term modeling uptake in Ω_1. The expression

(4.1) suggests that the reaction term is a superposition operator of the real function

$$G : \mathbb{R} \times \Omega \times [0,T] \to \mathbb{R}, \quad G(y_1, x, t) := \alpha \frac{y_1}{|y_1| + K_P} \frac{I(x', t)\mathrm{e}^{-x_3 K_W}}{|I(x', t)\mathrm{e}^{-x_3 K_W}| + K_I}. \tag{4.2}$$

Obviously, the functions $x \mapsto G(y_1, x, t)$ and $(x, t) \mapsto G(y_1, x, t)$ are measurable for every fixed $y_1 \in \mathbb{R}$ and, in the first case, $t \in [0, T]$. The function $y_1 \mapsto G(y_1, x, t)$ is continuous for almost every $(x, t) \in \Omega \times [0, T]$. Furthermore, Lemma 4.2.1 shows $|G(y_1, x, t)| \leq \alpha$ for all $y_1 \in \mathbb{R}, x \in \Omega$, and $t \in [0, T]$. Thus, the theorems 3.1 and 3.7 of Appell et Zabrejko [1] can be applied twice. First, we consider a fixed point of time $t \in [0, T]$. Then, the function $G(t) : \mathbb{R} \times \Omega \to \mathbb{R}$, $G(t)(y_1, x) := G(y_1, x, t)$ defines the continuous superposition operator $G(t) : L^2(\Omega) \to L^2(\Omega)$. Analogously, the real function G is associated with the continuous superposition operator $G : L^2(Q_T) \to L^2(Q_T)$. Obviously, the operator G is defined by the indexed family $(G(t))_t$ in the sense of Hypothesis 1.2.1. Henceforth, we will write $G(y_1, x, t)$ instead of both $G(t)(y_1)(x)$ and $G(y_1)(x, t)$ for all $y_1 \in L^2(\Omega)$ and $y_1 \in L^2(Q_T)$, respectively. We will adopt this notation for the operators E, $\bar{F}$, d, and b defined below as well.

Furthermore, the model describes the transformation of a fraction $\nu \in (0, 1)$ of the uptake G into y_2. The remnants are exported into Ω_2. For the sake of simplicity, it is assumed that the material of a whole water column enters Ω_2 at the same time, i.e., sinking processes in Ω_1 are neglected. The accumulated export at a fixed $t \in [0, T]$ is modeled by the nonlocal reaction term $E(t) : L^2(\Omega) \to L^2(\Omega')$ with

$$E(y_1, x', t) := (1 - \nu) \int_0^{h_e(x')} G(y_1, (x', x_3), t) dx_3 \qquad \text{for all } y_1 \in L^2(\Omega), x' \in \Omega'.$$

Proposition 4.2.3 at the end of Section 4.2.3 shows that $E(t)$ is well-defined and that the family $(E(t))_t$ defines an operator $E : L^2(Q_T) \to L^2(0, T; L^2(\Omega'))$ in the sense of Hypothesis 1.2.1.

Sinking through the lower layer, the export is remineralized into phosphate. The amount of remineralized export at $t \in [0, T]$ is described by $\bar{F}(t) : L^2(\Omega) \to L^2(\Omega_2)$ with

$$\bar{F}(y_1, x, t) := -E(y_1, x', t) \frac{\beta}{\bar{h}_e} \left(\frac{x_3}{\bar{h}_e} \right)^{-\beta - 1} \qquad \text{for all } y_1 \in L^2(\Omega), x \in \Omega_2.$$

This expression is equal to the derivative of $x_3 \mapsto E(y_1, x', t) \left(x_3 / \bar{h}_e \right)^{-\beta}$. The exponent $\beta > 0$ describes how remineralization responds to depth. Again Proposition 4.2.3 ensures that $\bar{F}(t)$ is well-defined and the family consisting of these operators defines the time-dependent operator $\bar{F} : L^2(Q_T) \to L^2(0, T; L^2(\Omega_2))$.

Summing up, the described processes, regarded at a fixed point of time $t \in [0, T]$, are represented by the nonlinear reaction term $d(t) : L^2(\Omega)^2 \to L^2(\Omega)^2$ with

$$d_1(y, x, t) := \begin{cases} -\lambda y_2(x) + G(y_1, x, t) & \text{if } x \in \Omega_1, \\ -\lambda y_2(x) + \bar{F}(y_1, x, t) & \text{if } x \in \Omega_2 \end{cases}$$

and

$$d_2(y, x, t) := \begin{cases} \lambda y_2(x) - \nu G(y_1, x, t) & \text{if } x \in \Omega_1, \\ \lambda y_2(x) & \text{if } x \in \Omega_2 \end{cases}$$

for all $y \in L^2(\Omega)^2$ and almost all $x \in \Omega$. The families $(G(t))_t$ and $(\bar{F}(t))_t$ define time-dependent operators in the sense of Hypothesis 1.2.1. The same is obviously true for $(\lambda Id)_t$. Thus, the family $(d(t))_t$ defines the reaction term $d : Y \to L^2(Q_T)^2$.

In Table 4.2.1, we provide a list of the *PO_4-DOP* model's parameters. They will be of interest in Chapter 5. The model features seven parameters which are all constant. Thus, the parameter space is equal to $U = \mathbb{R}^7$.

Table 4.2.1: The parameters of the *PO_4-DOP* model. The descriptions are partly taken from Prieß et al. [17].

Name	Description	Range
λ	remineralization rate of *DOP*	$\mathbb{R}_{>0}$
α	maximum uptake rate	$\mathbb{R}_{>0}$
K_P	half saturation constant of PO_4	$\mathbb{R}_{>0}$
K_I	half saturation constant of light	$\mathbb{R}_{>0}$
K_W	attenuation of water	$\mathbb{R}_{>0}$
β	sinking velocity exponent	$\mathbb{R}_{>0}$
ν	fraction of *DOP*	$(0, 1)$

4.2.3 Boundary conditions

The original formulation of the *PO_4-DOP* model lacks boundary conditions. Hence, this section is dedicated to the choice of an appropriate coupling term b on the boundary.

Since the *PO_4-DOP* model describes a cycle, possible solutions should have a constant mass. Theorem 1.5.3 and Remark 1.5.4 state that this is the case if the conservation of mass condition

$$\sum_{j=1}^{2} \left(\int_\Omega d_j(z, x, t)dx + \int_\Gamma b_j(z, \sigma, t)d\sigma \right) = 0$$

is fulfilled for every $z \in Y$ and almost every $t \in [0, T]$. We use this equality to derive an appropriate b for the *PO_4-DOP* model. To this end, we transform the integrals over the reaction terms d_j into boundary integrals.

Let $z \in Y$. The definition of d yields

$$\sum_{j=1}^{2} \int_{\Omega} d_j(z,x,t)dx = \int_{\Omega_1} G(z_1,x,t)dx - \int_{\Omega_2} E(z_1,x',t)\frac{\beta}{\bar{h}_e}\left(\frac{x_3}{\bar{h}_e}\right)^{-\beta-1} dx - \int_{\Omega_1} \nu G(z_1,x,t)dx.$$

The summands with λ cancel each other out. The last term on the right-hand side can be subtracted from the first. Because of the definition of Ω_2, the middle term is equal to

$$M := \int_{\Omega_2} E(z_1,x',t)dx_3\frac{\beta}{\bar{h}_e}\left(\frac{x_3}{\bar{h}_e}\right)^{-\beta-1} dx = \int_{\Omega_2'} E(z_1,x',t)\frac{\beta}{\bar{h}_e}\int_{\bar{h}_e}^{h(x')}\left(\frac{x_3}{\bar{h}_e}\right)^{-\beta-1} dx_3 dx'.$$

The integral with respect to x_3 is transformed into

$$\frac{\beta}{\bar{h}_e}\int_{\bar{h}_e}^{h(x')}\left(\frac{x_3}{\bar{h}_e}\right)^{-\beta-1} dx_3 = \left(\frac{1}{\bar{h}_e}\right)^{-\beta}\Big[-x_3^{-\beta}\Big]_{\bar{h}_e}^{h(x')} = \left(\frac{1}{\bar{h}_e}\right)^{-\beta}\Big[\bar{h}_e^{-\beta} - h(x')^{-\beta}\Big] = 1 - \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta}.$$

Therefore, M is equal to

$$M = \int_{\Omega_2'} E(z_1,x',t)dx' - \int_{\Omega_2'} E(z_1,x',t)\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta} dx'.$$

Because of $\Omega' = \Omega_1' \dot{\cup} \Omega_2'$, we obtain for the first summand

$$\int_{\Omega_2'} E(z_1,x',t)dx' = \int_{\Omega'} E(z_1,x',t)dx' - \int_{\Omega_1'} E(z_1,x',t)dx'.$$

Using the definitions of E and Ω_1, the integral over Ω' can be transformed into

$$\int_{\Omega'} E(z_1,x',t)dx' = (1-\nu)\int_{\Omega'}\int_0^{h_e(x')} G(z_1,(x',x_3),t)dx_3dx' = (1-\nu)\int_{\Omega_1} G(z_1,x,t)dx.$$

Combining the results, we arrive at

$$\sum_{j=1}^{2} \int_{\Omega} d_j(z,x,t)dx = \int_{\Omega_1'} E(z_1,x',t)dx' + \int_{\Omega_2'} E(z_1,x',t)\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta} dx'$$

which implies that the boundary reaction term b should fulfill

$$\sum_{j=1}^{2} \int_{\Gamma} b_j(z,\sigma,t)d\sigma = -\int_{\Omega_1'} E(z_1,x',t)dx' - \int_{\Omega_2'} E(z_1,x',t)\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta} dx'$$

for every $z \in Y$ to comply with the conservation of mass condition. This equation is fulfilled by the boundary reaction term $b(t) : L^2(\Omega)^2 \to L^2(\Gamma)^2$ at a fixed $t \in [0,T]$, defined by

$b_2(t) = 0$ and

$$b_1(y,x,t) := \begin{cases} -E(y_1, x', t) & \text{if } x = (x', h(x')) \in \Gamma_1, \\ -E(y_1, x', t)\left(\dfrac{h(x')}{\bar{h}_e}\right)^{-\beta} & \text{if } x = (x', h(x')) \in \Gamma_2, \\ 0 & \text{if } x = (x', 0) \in \Gamma' \end{cases}$$

for all $y \in L^2(\Omega)^2$ and almost all $x \in \Gamma$. Proposition 4.2.3 ensures that the family $(b(t))_t$ defines the boundary reaction term $b : Y \to L^2(\Sigma)^2$ in the sense of Hypothesis 1.2.1.

In summary, we obtain the following result for the *PO*$_4$-*DOP* model.

Result 4.2.2. *The spaces* $\Lambda = L^2(\Omega)^2$ *and* $Y = L^2(Q_T)^2$*, the reaction terms* d *and* b*, and the right-hand sides* q_{Q_T} *and* q_Σ *of the PO*$_4$*-DOP model are in accordance with Hypothesis 1.2.1. Furthermore, reaction terms and right-hand sides fulfill the conservation of mass conditions of Remark 1.5.4.*

The final proposition provides estimates for the reaction terms.

Proposition 4.2.3. *There exists a constant* $M_{GEF} > 0$ *such that*

$$\max\{\|G(y_1(t))\|_{L^2(\Omega_1)}, \|E(y_1(t))\|_{L^2(\Omega')}, \|\bar{F}(y_1(t))\|_{L^2(\Omega_2)}, \|b_1(y(t))\|_{L^2(\Gamma)}\} \leq M_{GEF}$$

holds for all $y \in L^2(Q_T)^2, t \in [0,T]$.

Proof. First, we observe that the coordinate indicating depth x_3 belongs to $(\bar{h}_e, h(x')]$ if $(x', x_3) \in \Omega_2 \cup \Gamma_2$. Given an arbitrary $\gamma > 0$, we conclude

$$\left(\frac{x_3}{\bar{h}_e}\right)^{-\gamma} = \left(\frac{\bar{h}_e}{x_3}\right)^{\gamma} \leq \left(\frac{\bar{h}_e}{\bar{h}_e}\right)^{\gamma} = 1 \quad \text{for all } (x', x_3) \in \Omega_2 \cup \Gamma_2. \tag{4.3}$$

Let $y \in L^2(Q_T)^2$ and $t \in [0,T]$. The estimate for G relies on Lemma 4.2.1. Using result and notation of this lemma, we obtain

$$\|G(y_1(t))\|^2_{L^2(\Omega_1)} = \int_{\Omega_1} \left[\alpha f_{K_P}(y_1(t)) f_{K_I}(I(t)\mathrm{e}^{-x_3 K_W})\right]^2 dx \leq \alpha^2 |\Omega_1|.$$

Regarding E, we estimate G as before. Using additionally $h_e(x') \leq \bar{h}_e$, we arrive at

$$\|E(y_1(t))\|^2_{L^2(\Omega')} = \int_{\Omega'} (1-\nu)^2 \left[\int_0^{h_e(x')} G(y_1, (x', x_3), t) dx_3\right]^2 dx \leq \alpha^2 \bar{h}_e^2 (1-\nu)^2 |\Omega'|.$$

As to $\bar{F}$, we estimate the fraction by Equation (4.3) and treat E as above. We obtain

$$\|\bar{F}(y_1(t))\|^2_{L^2(\Omega_2)} = \int_{\Omega_2} \left[E(y_1, x', t)\frac{\beta}{\bar{h}_e}\left(\frac{x_3}{\bar{h}_e}\right)^{-\beta-1}\right]^2 dx \leq |\Omega_2| \alpha^2 \bar{h}_e^2 (1-\nu)^2 \frac{\beta^2}{\bar{h}_e^2}.$$

Finally, the definition of b_1 and Equation (4.3) yield

$$\|b_1(y(t))\|_{L^2(\Gamma)}^2 = \int_{\Omega_1'} E(y_1, x', t)^2 dx' + \int_{\Omega_2'} E(y_1, x', t)^2 \left(\frac{h(x')}{\bar{h}_e}\right)^{-2\beta} dx' \leq \|E(y_1(t))\|_{L^2(\Omega')}^2.$$

Thus, the proposition's assertion holds with $M_{GEF} := \alpha \max\{\sqrt{|\Omega_1|}, \bar{h}_e(1-\nu)\sqrt{|\Omega'|}, (1-\nu)\beta\sqrt{|\Omega_2|}\}$. □

4.3 The iron equation

The *PO_4-DOP-Fe* model describes how the phosphorus cycle reacts to a variable concentration of iron. As the name implies, the model considers the $s = 3$ constituents phosphate, dissolved organic phosphorus, and iron. The concentrations of PO_4 and DOP, y_1 and y_2, are modeled by the two equations of the *PO_4-DOP* model adapted to the variable iron concentration y_3. The uptake of phosphate, represented by the operator G, is the only reaction that is influenced by iron. Thus, in the context of the *PO_4-DOP-Fe* model, we regard G in the form of Equation (4.1) depending on y_1 and y_3. The corresponding superposition operators $G(t)$ and G, now defined on $L^2(\Omega)^2$ and $L^2(Q_T)^2$, respectively, fulfill the same properties as the original ones, defined on $L^2(\Omega)$ and $L^2(Q_T)$, because the saturation function for iron is bounded by 1 according to Lemma 4.2.1. Similarly, all properties of E, $\bar{F}$, d, and b remain valid if their domain of definition is extended accordingly.

The concentration of iron y_3 is characterized by

$$\begin{aligned} \partial_t y_3 + \mathbf{v} \cdot \nabla y_3 - \operatorname{div}(\kappa \nabla y_3) + d_3(y, x, t) &= q_{Q_T 3} \quad \text{in } Q_T \\ \nabla y_3 \cdot (\kappa \eta) + b_3(y, x, t) &= q_{\Sigma 3} \quad \text{in } \Sigma. \end{aligned} \tag{4.4}$$

This and the following section is dedicated to the definition of d_3, b_3, $q_{Q_T 3}$, and $q_{\Sigma 3}$.

We deal with the right-hand sides first. Unlike the other constituents, iron is supplied by an external source $q_{Q_T 3} \in L^2(Q_T)$. This term, describing an aeolian source of iron, is nonzero only in the euphotic zone. The right-hand side on the boundary is zero, i.e., $q_{\Sigma 3} = 0$.

The reaction term d_3 considers the influence of the phosphorus cycle, complexation, and scavenging. We deal with the last two phenomena in a separate section. The phosphorus cycle causes an increase of the iron concentration due to remineralization and a decrease due to consumption. A multiplication with the constant ratio $R_{Fe} > 0$ turns phosphorus units into iron units. Thus, iron increases by $\lambda y_2 R_{Fe}$ in Ω and decreases by $G(y_1, y_3) R_{Fe}$ in Ω_1.

We formulate the complete reaction terms d_3 and b_3 at the end of the next section after introducing scavenging and complexation.

4.3.1 Scavenging and complexation

Scavenging provides an additional sink of iron. Since only free iron is subject to scavenging, this reaction is influenced by the complexation of iron with organic ligand. We consider complexation by splitting the total iron concentration y_3 into free iron Fe' and complexed iron FeL. Similarly, the amount of total ligand L_T is the sum of free ligand L' and complexed ligand. The amount of the latter is equal to the complexed iron FeL. These relations are formally expressed by $y_3 = Fe' + FeL$ and $L_T = L' + FeL$. Parekh et al. [15] assume that the total ligand concentration is constant.

The reaction term for scavenging, referred to as J_{Fe}, is given by the first order loss process $J_{Fe} := k_{sc}Fe'$. The scavenging rate k_{sc} determines the part of free iron that is subject to scavenging. The rate depends on the available particle concentration and thus varies with depth. Parekh et al. assume that k_{sc} is positive and belongs to $L^\infty(Q_T)$.

Hypothesis 1.2.1 requires J_{Fe} to depend at least on one of the concentrations y_1, y_2 or y_3. Therefore, we express Fe' as a function of y_3 using the equilibrium relationship $K = FeL/(Fe'L')$ with a constant $K > 0$ (cf. Parekh et al. [15, Section 2.3]). To begin with, we assume that all appearing concentrations are real numbers and, additionally, that Fe' and L' are nonzero.

Inserting the expression $L' = FeL/(KFe')$, an equivalent of the equilibrium relationship, into the equation for ligand, we obtain

$$L_T = FeL + L' = FeL + \frac{FeL}{KFe'} = FeL\left(1 + \frac{1}{KFe'}\right).$$

The quantity FeL can be replaced by $y_3 - Fe'$. This gives

$$L_T = (y_3 - Fe')\left(1 + \frac{1}{KFe'}\right) = y_3 - Fe' + \frac{y_3}{KFe'} - \frac{1}{K}.$$

With the abbreviation $H(y_3) := L_T + 1/K - y_3$, this proves equivalent to

$$Fe'^2 + H(y_3)Fe' - \frac{y_3}{K} = 0.$$

Thus, we obtain a relationship between Fe' and y_3. To ensure that the solutions of the quadratic equation are real, we prove that the expression $r := (L_T + 1/K - y_3)^2/4 + y_3/K$ is positive. This is obvious whenever y_3 is nonnegative. In the negative case, we transform r into

$$\begin{aligned} r &= \frac{1}{4}\left(L_T + \frac{1}{K} - y_3\right)^2 + \frac{y_3}{K} \\ &= \frac{1}{4}\left(L_T + \frac{1}{K}\right)^2 - \frac{1}{2}\left(L_T + \frac{1}{K}\right)y_3 + \frac{1}{4}y_3^2 + \frac{y_3}{K} \\ &= \frac{1}{4}\left(L_T + \frac{1}{K}\right)^2 + \frac{1}{4}y_3^2 - \frac{1}{2}y_3\left(L_T - \frac{1}{K}\right). \end{aligned}$$

Parekh et al. set $K = \exp(11)$ and $L_T = 1$. Therefore, it is reasonable to assume that $L_T - 1/K$ is nonnegative. Under this assumption, $y_3 < 0$ implies $-y_3(L_T - 1/K)/2 \geq 0$ and, as a consequence, $r > 0$.

It is known that the quadratic equation for Fe' has the two solutions

$$Fe'_1(y_3) = -\frac{1}{2}H(y_3) + \sqrt{\frac{H(y_3)^2}{4} + \frac{y_3}{K}} \quad \text{and} \quad Fe'_2(y_3) = -\frac{1}{2}H(y_3) - \sqrt{\frac{H(y_3)^2}{4} + \frac{y_3}{K}}$$

which are both real because the radicand r is positive. In the following lemma, we prove that the second solution is unsuited for describing a concentration.

Lemma 4.3.1. *The function Fe'_2 maps $\mathbb{R}$ into $\mathbb{R}_{<0}$.*

Proof. Let $\tilde{y}_3 \in \mathbb{R}$ with $\tilde{y}_3 < L_T + 1/K$. Since the square root is nonnegative, we conclude $Fe'_2(\tilde{y}_3) \leq -(L_T + 1/K - \tilde{y}_3)/2 < 0$. Thus, Fe'_2 has negative values.

To show that Fe'_2 has only negative values, we argue by contradiction. Suppose that Fe'_2 had a nonnegative value. Then, the intermediate value theorem yields a root of the continuous function Fe'_2, i.e., an element $y_3 \in \mathbb{R}$ with

$$-\frac{1}{2}\left(L_T + \frac{1}{K} - y_3\right) = \sqrt{\frac{1}{4}\left(L_T + \frac{1}{K} - y_3\right)^2 + \frac{y_3}{K}}.$$

Squaring both sides, we obtain $(L_T + 1/K - y_3)^2/4 = (L_T + 1/K - y_3)^2/4 + y_3/K$ and therefore $y_3 = 0$. However, because of $0 < L_T + 1/K$, the first statement of this proof yields $Fe'_2(y_3) = Fe'_2(0) < 0$. This contradicts the property that y_3 is a root. □

Because of the monotonicity of the square root function, the first solution Fe'_1 is nonnegative for all input values $y_3 \geq 0$ and otherwise negative. Thus, only unrealistic input values (negative concentrations of total iron) cause unrealistic output values (negative concentrations of free iron). For this reason, we will use $Fe' := Fe'_1$ in the following definition of J_{Fe}.

To define the reaction term J_{Fe} for scavenging, let $k_{sc} \in L^\infty(Q_T)$ be nonnegative almost everywhere. Furthermore, we choose $K > 0$ and $L_T \in L^\infty(Q_T)$ in such a way that $L_T \geq 1/K$ holds almost everywhere. The values Parekh et al. [15] use for K and L_T fulfill this property. However, we admit a variable concentration of total ligand.

To ensure that the real function Fe' is associated with a superposition operator from $L^2(Q_T)$ to $L^2(Q_T)$, we show that $y_3 \in L^2(Q_T)$ implies

$$Fe'(y_3) = -\frac{1}{2}\left(L_T + \frac{1}{K} - y_3\right) + \sqrt{\frac{1}{4}\left(L_T + \frac{1}{K} - y_3\right)^2 + \frac{y_3}{K}} \quad \in L^2(Q_T).$$

The first summand is quadratically integrable because of the choice of y_3 and L_T. The radicand belongs to $L^1(Q_T)$ since $(L_T + 1/K - y_3) \in L^2(Q_T)$ and, in particular, $y_3/K \in L^1(Q_T)$. As a consequence, the square root belongs to $L^2(Q_T)$. We conclude $Fe'(y_3) \in L^2(Q_T)$. For almost every t, the same arguments with Q_T replaced by Ω show that $Fe'(t)$:

$L^2(\Omega) \to L^2(\Omega)$, given by

$$Fe'(t)(v_3) = -\frac{1}{2}\left(L_T(t) + \frac{1}{K} - v_3\right) + \sqrt{\frac{1}{4}\left(L_T(t) + \frac{1}{K} - v_3\right)^2 + \frac{v_3}{K}} \quad \text{for all } v_3 \in L^2(\Omega),$$

is well-defined as well.

Using the preliminary results, we define the reaction term for scavenging and complexation $J_{Fe} : L^2(Q_T) \to L^2(Q_T)$ by

$$J_{Fe}(y_3) := k_{sc} Fe'(y_3) \quad \text{for all } y_3 \in L^2(Q_T)$$

as well as the operators $J_{Fe}(t) = k_{sc}(t)Fe'(t)$ for almost every t. Obviously, the family $(J_{Fe}(t))_t$ is associated with J_{Fe} in the sense of Hypothesis 1.2.1.

Finally, we provide the complete reaction terms of the PO_4-DOP-Fe model. The reaction terms are defined on the domain of definition $Y = L^2(Q_T)^3$ and the generating families on $\Lambda = L^2(\Omega)^3$. Obviously, these spaces fulfill the condition (1.1). Concerning boundary conditions for iron, we observe that it is not appropriate to claim conservation of mass because of the nontrivial source term $q_{Q_T 3}$. Since the source of iron is not defined via a boundary condition, we choose homogeneous Neumann boundary conditions for y_3.

Definition 4.3.2 (The PO_4-DOP-Fe model)**.** *Let $Y := L^2(Q_T)^3$ and $\Lambda := L^2(\Omega)^3$. The reaction term $d : Y \to L^2(Q_T)^3$ is defined by the family $(d(t))_t$ consisting of operators $d(t) : \Lambda \to L^2(\Omega)^3$ with the components*

$$d_1(y, x, t) := \begin{cases} -\lambda y_2(x) + G(y_1, y_3, x, t) & \text{if } x \in \Omega_1, \\ -\lambda y_2(x) + \bar{F}(y_1, y_3, x, t) & \text{if } x \in \Omega_2, \end{cases}$$

$$d_2(y, x, t) := \begin{cases} \lambda y_2(x) - \nu G(y_1, y_3, x, t) & \text{if } x \in \Omega_1, \\ \lambda y_2(x) & \text{if } x \in \Omega_2, \end{cases}$$

and

$$d_3(y, x, t) := \begin{cases} -\lambda y_2(x) R_{Fe} + J_{Fe}(y_3, x, t) + G(y_1, y_3, x, t) R_{Fe} & \text{if } x \in \Omega_1, \\ -\lambda y_2(x) R_{Fe} + J_{Fe}(y_3, x, t) & \text{if } x \in \Omega_2 \end{cases}$$

for all $y \in \Lambda$, almost all $x \in \Omega$, and almost all $t \in [0, T]$.

The boundary reaction term $b : Y \to L^2(\Sigma)^3$ is defined by the family $(b(t))_t$ consisting of $b(t) : \Lambda \to L^2(\Gamma)^3$ with the components $b_2(t) = b_3(t) = 0$ and

$$b_1(y, x, t) := \begin{cases} -E(y_1, y_3, x', t) & \text{for } x = (x', h(x')) \in \Gamma_1, \\ -E(y_1, y_3, x', t)\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta} & \text{for } x = (x', h(x')) \in \Gamma_2, \\ 0 & \text{for } x = (x', 0) \in \Gamma' \end{cases}$$

for all $y \in \Lambda$, almost all $x \in \Gamma$, and almost all $t \in [0,T]$.

The right-hand side $q_{Q_T} \in L^2(Q_T)^3$ consists of the components $q_{Q_T1} = q_{Q_T2} = 0$ and $q_{Q_T3} \in L^2(Q_T)$ with $q_{Q_T3}(x,t) = 0$ for almost all $(x,t) \in \Omega_2 \times [0,T]$. On the boundary, we assume $q_\Sigma = 0 \in L^2(\Sigma)^3$.

4.4 Application of the existence theorems

4.4.1 Transient solutions of the PO_4-DOP-Fe model and the PO_4-DOP model

Let $y_0 \in L^2(\Omega)^3$ be an initial value. In this section, we apply Theorem 2.3.2 to prove that the PO_4-DOP-Fe model has a unique transient solution.

The reaction terms and right-hand sides, given in Definition 4.3.2, fulfill Hypothesis 1.2.1. The same is true for the domains of definition $Y = L^2(Q_T)^3$ and $\Lambda = L^2(\Omega)^3$ since $W(0,T)^3$ is continuously embedded in Y and the condition (1.1) is fulfilled.

We define the operator $F_1 : Y \to L^2(0,T;H^1(\Omega)^*)^3$ by means of the reaction terms and $f \in L^2(0,T;H^1(\Omega)^*)^3$ by means of the right-hand sides according to Lemma 1.4.1. Moreover, let $F_2 = 0$. Thus, Hypothesis 2.1.1 is fulfilled with $Y_1 = Y_2 = Y$.

The rest of this section is dedicated to the remaining assumptions of the existence theorem 2.3.2. Clearly, $C([0,T];L^2(\Omega))^3$ is continuously embedded in Y. Furthermore, $d(0) = b(0) = 0$ because the components λId, G, E, $\bar{F}$, and Fe' all fulfill this property. This implicates that F_1 is homogeneous. Regarding the Lipschitz condition for $F_1(t)$, Lemma 1.4.1 yields

$$\|F_1(y(t)) - F_1(z(t))\|_{(H^1(\Omega)^*)^3} \le \|d(y,.,t) - d(z,.,t)\|_{\Omega^3} + c_\tau \|b(y,.,t) - b(z,.,t)\|_{\Gamma^3}$$

for all $y, z \in Y$ and almost all t. Thus, it suffices to prove the required Lipschitz condition for $d(t)$ and $b(t)$ instead of $F_1(t)$.

Let t be a suitable element of $[0,T]$ and $y, z \in L^2(Q_T)^3$. As a preparation, we prove the Lipschitz condition for $G, E, \bar{F}$ and J_{Fe}. We will leave out some arguments of the appearing integrands (mostly x and t) for the sake of shortness. Employing notation and result of Lemma 4.2.1, we obtain

$$\begin{aligned}
\|G(y_1,y_3,.,t) - G(z_1,z_3,.,t)\|_\Omega^2 &\le \int_\Omega \alpha^2 f_{K_I}^2(I\mathrm{e}^{-x_3 K_W})[f_{K_P}(y_1)f_{K_F}(y_3) - f_{K_P}(z_1)f_{K_F}(z_3)]^2 dx \\
&\le \int_\Omega \alpha^2 \left[f_{K_P}(y_1)|f_{K_F}(y_3) - f_{K_F}(z_3)| + f_{K_F}(z_3)|f_{K_P}(y_1) - f_{K_P}(z_1)|\right]^2 dx \\
&\le \int_\Omega \alpha^2 \left[\frac{1}{K_F}|y_3(x,t) - z_3(x,t)| + \frac{1}{K_P}|y_1(x,t) - z_1(x,t)|\right]^2 dx \\
&\le 2\alpha^2 \max\left\{\frac{1}{K_P^2}, \frac{1}{K_F^2}\right\} \left[\|y_1(t) - z_1(t)\|_\Omega^2 + \|y_3(t) - z_3(t)\|_\Omega^2\right] \\
&\le L_G^2 \|y(t) - z(t)\|_{L^2(\Omega)^3}^2
\end{aligned}$$

with the Lipschitz constant $L_G := \sqrt{2}\alpha \max\{K_P^{-1}, K_F^{-1}\}$.

Regarding the export, we apply Hölder's inequality to the integral over $[0, h_e(x')]$ in the definition of E. Since $h_e(x') \le \bar{h}_e$ and the latter is independent of x', we arrive at the norm of $L^1(\Omega_1)$ in the third line of the following estimate. Finally, we employ the Lipschitz property of G. All in all, we obtain

$$\begin{aligned}
\|E(y_1, y_3, ., t) - E(z_1, z_3, ., t)\|_{\Omega'}^2 &= \int_{\Omega'} (1-\nu)^2 \left(\int_0^{h_e(x')} [G(y_1, y_3) - G(z_1, z_3)] dx_3 \right)^2 dx' \\
&\le (1-\nu)^2 \int_{\Omega'} h_e(x') \int_0^{h_e(x')} [G(y_1, y_3, x, t) - G(z_1, z_3, x, t)]^2 dx_3 dx' \\
&\le (1-\nu)^2 \bar{h}_e \|G(y_1, y_3, ., t) - G(z_1, z_3, ., t)\|_{\Omega_1}^2 \\
&\le (1-\nu)^2 \bar{h}_e L_G^2 \|y(t) - z(t)\|_{L^2(\Omega)^3}^2.
\end{aligned}$$

Next, we consider $\bar{F}$. This reaction term is bounded independently of x_3 because of (4.3). Thus, the integral over $[\bar{h}_e, h(x')]$ is equal to the difference $h(x') - \bar{h}_e$. In the third line of the following estimate, $h(x')$ is estimated by the constant maximum depth, and the remaining integral over Ω_2' is written as a norm. Finally, since $\Omega_2' \subseteq \Omega'$, the Lipschitz property of E can be employed. These arguments lead to

$$\begin{aligned}
\|\bar{F}(y_1, y_3, ., t) - \bar{F}(z_1, z_3, ., t)\|_{\Omega_2}^2 &= \int_{\Omega_2'} \int_{\bar{h}_e}^{h(x')} \frac{\beta^2}{\bar{h}_e^2} \left(\frac{x_3}{\bar{h}_e} \right)^{-2(\beta+1)} (E(y_1, y_3) - E(z_1, z_3))^2 dx_3 dx' \\
&\le \int_{\Omega_2'} \frac{\beta^2}{\bar{h}_e^2} (h(x') - \bar{h}_e)(E(y_1, y_3) - E(z_1, z_3))^2 dx' \\
&\le \frac{\beta^2}{\bar{h}_e^2} (h_{\max} - \bar{h}_e) \|E(y_1, y_3, ., t) - E(z_1, z_3, ., t)\|_{\Omega_2'}^2 \\
&\le \beta^2 \left(\frac{h_{\max}}{\bar{h}_e} - 1 \right) (1-\nu)^2 L_G^2 \|y(t) - z(t)\|_{L^2(\Omega)^3}^2.
\end{aligned}$$

At last, we treat the reaction term for scavenging J_{Fe}. To this end, we prove the Lipschitz continuity of the function $Fe' : \mathbb{R} \to \mathbb{R}$.

Lemma 4.4.1. *Let $(x, t) \in Q_T$ such that $L_T(x, t) \ge 1/K$ and $L_T := L_T(x, t)$. Then, the real function $Fe' : \mathbb{R} \to \mathbb{R}$, defined by*

$$Fe'(y_3) = -\frac{1}{2} \left(L_T + \frac{1}{K} - y_3 \right) + \sqrt{\frac{1}{4} \left(L_T + \frac{1}{K} - y_3 \right)^2 + \frac{y_3}{K}},$$

is Lipschitz continuous, and $L_F := 1$ is a Lipschitz constant. In particular, the Lipschitz constant is independent of t.

Proof. Because of the mean value theorem for differentiable real functions, it suffices to prove that the first derivative of Fe' is bounded by 1. This derivative exists because Fe' is composed of differentiable functions. Given $y_3 \in \mathbb{R}$, the usual differentiation rules yield

$$d_{y_3} Fe'(y_3) = \frac{1}{2}\left(1 + \frac{\frac{1}{2}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right) + \frac{1}{K}}{\sqrt{\frac{1}{4}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right)^2 + \frac{y_3}{K}}}\right).$$

Referring to the fraction as Φ, we obtain the abridged notation $d_{y_3} Fe'(y_3) = (1+\Phi)/2$. First, we prove $\Phi \in [-1, 1]$ for all $y_3 \in \mathbb{R}$. To this end, we distinguish between two cases for y_3. For the sake of shortness, we abbreviate $M_{KL} := L_T + 1/K$.

In the first case, we assume $y_3 < L_T - 1/K$. This assumption ensures that the numerator and therefore the whole fraction Φ is negative, i.e., bounded from above by zero. The following transformations show that it is bounded from below as well. In the first step, suitable summands are added on both sides of the clearly true first inequality. Then, we apply the binomial identity and extract the square root which is bijective on the nonnegative real numbers. We obtain

$$\begin{aligned}
& & -\frac{L_T}{K} &\leq 0 \\
&\iff & \frac{1}{4}(y_3 - M_{KL})^2 + \frac{1}{K}(y_3 - M_{KL}) + \frac{1}{K^2} &\leq \frac{1}{4}(y_3 - M_{KL})^2 + \frac{y_3}{K} \\
&\iff & \left(\frac{1}{2}(y_3 - M_{KL}) + \frac{1}{K}\right)^2 &\leq \frac{1}{4}(y_3 - M_{KL})^2 + \frac{y_3}{K} \\
&\iff & \left|\frac{1}{2}(y_3 - M_{KL}) + \frac{1}{K}\right| &\leq \sqrt{\frac{1}{4}(y_3 - M_{KL})^2 + \frac{y_3}{K}} \\
&\iff & -\left(\frac{1}{2}(y_3 - M_{KL}) + \frac{1}{K}\right) &\leq \sqrt{\frac{1}{4}(y_3 - M_{KL})^2 + \frac{y_3}{K}}.
\end{aligned}$$

In the last line, we use that the numerator of Φ is negative according to the choice of y_3. The last inequality is equivalent to $\Phi \geq -1$. Therefore, $\Phi \in [-1, 0]$.

In the second case, we assume $y_3 \geq L_T - 1/K$. Under this assumption, the numerator of Φ is nonnegative. Thus, it can be written as a square root. Further transformations yield

$$\begin{aligned}
\Phi &= \sqrt{\frac{\left(\frac{1}{2}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right) + \frac{1}{K}\right)^2}{\frac{1}{4}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right)^2 + \frac{y_3}{K}}} = \sqrt{\frac{\frac{1}{4}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right)^2 + \left(y_3 - \left(L_T + \frac{1}{K}\right)\right)\frac{1}{K} + \frac{1}{K^2}}{\frac{1}{4}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right)^2 + \frac{y_3}{K}}} \\
&= \sqrt{1 - \frac{\frac{L_T}{K}}{\frac{1}{4}\left(y_3 - \left(L_T + \frac{1}{K}\right)\right)^2 + \frac{y_3}{K}}}.
\end{aligned}$$

We abbreviate the expression beneath the last square root by $1 - \Psi$ and show that it belongs to $[0, 1]$.

The numerator of Ψ is nonnegative because of the assumptions $L_T \geq 1/K$ and $K > 0$. The denominator is equal to the positive expression r which was defined and investigated on page 60. As a consequence, the fraction Ψ is nonnegative and thus $1 - \Psi \leq 1$. In addition, the computation above shows that $1 - \Psi$ equals $((y_3 - (L_T + \frac{1}{K}))/2 + 1/K)^2/r$ which is clearly nonnegative. We conclude $1-\Psi \in [0,1]$.

From this it follows that $\Phi = \sqrt{1-\Psi}$ belongs to $[0,1]$ under the assumption of the second case.

Combining both cases, we obtain $\Phi \in [-1,1]$ for every $y_3 \in \mathbb{R}$. In particular, $1+\Phi \geq 0$ and $\Phi \leq 1$. Both facts ensure that the estimate

$$\left|d_{y_3} Fe'(y_3)\right| = \left|\frac{1}{2}(1+\Phi)\right| = \frac{1}{2}(1+\Phi) \leq \frac{1}{2}(1+1) = 1$$

holds for all $y_3 \in \mathbb{R}$. Thus, the mean value theorem yields the Lipschitz continuity of Fe' with the Lipschitz constant $L_F = 1$. □

The lemma and the definition of J_{Fe} yield the desired estimate

$$\|J_{Fe}(y_3,.,t) - J_{Fe}(z_3,.,t)\|_\Omega^2 \leq \|k_{sc}\|^2_{L^\infty(Q_T)} L_F^2 \|y(t)-z(t)\|^2_{L^2(\Omega)^3}.$$

In the next step, we employ the preparatory results to prove the Lipschitz conditions for d and b. As to d_1, the triangle inequality in combination with the convexity of the square function on yields

$$\begin{aligned}
&\|d_1(y,.,t) - d_1(z,.,t)\|_\Omega^2 \\
&\quad \leq 3\left(\lambda^2\|y_2(t)-z_2(t)\|_\Omega^2 + \|G(y_1,y_3,t)-G(z_1,z_3,t)\|_{\Omega_1}^2 + \|\bar{F}(y_1,y_3,t)-\bar{F}(z_1,z_3,t)\|_{\Omega_2}^2\right) \\
&\quad \leq 3\left(\lambda^2\|y_2(t)-z_2(t)\|_\Omega^2 + L_G^2\left(1+\left(\frac{h_{\max}}{\bar{h}_e}-1\right)\beta^2(1-\nu)^2\right)\|y(t)-z(t)\|_{\Omega^3}^2\right) \\
&\quad \leq 3\left(\lambda^2 + L_G^2\left(1+\left(\frac{h_{\max}}{\bar{h}_e}-1\right)\beta^2(1-\nu)^2\right)\right)\|y(t)-z(t)\|_{\Omega^3}^2.
\end{aligned}$$

Concerning d_2, we similarly conclude

$$\begin{aligned}
\|d_2(y,.,t) - d_2(z,.,t)\|_\Omega^2 &\leq 2\left(\lambda^2\|y_2(t)-z_2(t)\|_\Omega^2 + \nu^2\|G(y_1,y_3,t)-G(z_1,z_3,t)\|_{\Omega_1}^2\right) \\
&\leq 2\left(\lambda^2 + L_G^2\nu^2\right)\|y(t)-z(t)\|_{\Omega^3}^2.
\end{aligned}$$

Finally, we obtain for the third component

$$\begin{aligned}
&\|d_3(y,.,t) - d_3(z,.,t)\|_\Omega^2 \\
&\qquad \leq 3\left(\lambda^2 R_{Fe}^2\|y_2(t)-z_2(t)\|_\Omega^2 + R_{Fe}^2\|G(y_1,y_3)-G(z_1,z_3)\|_{\Omega_1}^2 + \|J_{Fe}(y_3)-J_{Fe}(z_3)\|_\Omega^2\right) \\
&\qquad \leq 3\left(\lambda^2 R_{Fe}^2\|y_2(t)-z_2(t)\|_\Omega^2 + \left(L_G^2 R_{Fe}^2 + \|k_{sc}\|^2_{L^\infty(Q_T)}L_F^2\right)\|y(t)-z(t)\|_{\Omega^3}^2\right) \\
&\qquad \leq 3\left(\lambda^2 R_{Fe}^2 + L_G^2 R_{Fe}^2 + \|k_{sc}\|^2_{L^\infty(Q_T)}L_F^2\right)\|y(t)-z(t)\|_{\Omega^3}^2.
\end{aligned}$$

Hence, the operator $d(t): L^2(\Omega)^3 \to L^2(\Omega)^3$ is Lipschitz continuous. The Lipschitz constant L_d is equal to the sum of the constants for $d_j(t)$, $j \in \{1,2,3\}$, and thus independent of t.

The nonlinear boundary reaction term b_1 is treated similarly. By definition, the euphotic boundary Γ_1 corresponds to Ω_1' and the aphotic boundary Γ_2 to Ω_2'. Using Equation (4.3) with $\gamma := 2\beta$ and the Lipschitz continuity of $E(t)$, we obtain

$$\begin{aligned}
&\|b_1(y, ., t) - b_1(z, ., t)\|_\Gamma^2 \\
&\quad = \int_{\Omega_1'} (E(y_1, y_3) - E(z_1, z_3))^2 dx' + \int_{\Omega_2'} (E(y_1, y_3) - E(z_1, z_3))^2 \left(\frac{h(x')}{\bar{h}_e}\right)^{-2\beta} dx' \\
&\quad \leq \|E(y_1, y_3, ., t) - E(z_1, z_3, ., t)\|_{\Omega'}^2 \leq (1-\nu)^2 \bar{h}_e L_G^2 \|y(t) - z(t)\|_{\Omega^3}^2.
\end{aligned}$$

Since $b_2 = b_3 = 0$, the complete reaction term $b(t) : L^2(\Omega)^3 \to L^2(\Gamma)^3$ is Lipschitz continuous. The Lipschitz constant L_b is equal to the one for b_1 and thus independent of t.

In summary, the reaction terms of the *PO*$_4$-*DOP*-*Fe* model, given in Definition 4.3.2, fulfill the assumptions of Theorem 2.3.2. Therefore, this model has a unique transient solution with the initial value $y_0 \in L^2(\Omega)^3$. In particular, the *PO*$_4$-*DOP* model, defined in the sections 4.2.2 and 4.2.3, has a unique transient solution for each initial value $y_0 \in L^2(\Omega)^2$.

4.4.2 Periodic solutions of the *PO*$_4$-*DOP* model

Let $C \in \mathbb{R}$. In this section, we employ Theorem 3.2.1 to find a periodic solution with the constant mass C of the *PO*$_4$-*DOP* model.

The reaction terms, introduced in the sections 4.2.2 and 4.2.3, fulfill Hypothesis 1.2.1 with $Y = L^2(Q_T)^2$ and $\Lambda = L^2(\Omega)^2$ according to Result 4.2.2. To comply with the notation of Section 3.1, we assume that the operator $F : Y \to L^2(0,T;H^1(\Omega)^*)^2$ consists of the components F_1, defined by $d_1 + \lambda Id$ and b_1 in the sense of Lemma 1.4.1, and F_2, defined by $d_2 - \lambda Id$. Furthermore, we regard the right-hand side $f = 0 \in L^2(0,T;H^1(\Omega)^*)^2$. Since, in addition, $W(0,T)^2$ is compactly embedded in Y (see Růžička [19, Lemma 3.74]), and $\lambda > 0$ holds by assumption, all statements of Hypothesis 3.1.1 are satisfied. In particular, the *PO*$_4$-*DOP* model belongs to the class of models of *N*-*DOP* type.

The next three paragraphs address the remaining assumptions of Theorem 3.2.1.

Continuity. Section 4.4.1 yields the Lipschitz continuity of the *PO*$_4$-*DOP* model's reaction terms $d(t)$ and $b(t)$ with time-independent Lipschitz constants L_d and L_b. Thus, we obtain for the time-dependent operator $d : L^2(Q_T)^2 \to L^2(Q_T)^2$

$$\|d(y) - d(z)\|_{Q_T^2}^2 \leq \int_0^T \|d(y, ., t) - d(z, ., t)\|_{\Omega^2}^2 dt \leq L_d^2 \int_0^T \|y(t) - z(t)\|_{\Omega^2}^2 dt = L_d^2 \|y - z\|_{Q_T^2}^2$$

for all $y, z \in L^2(Q_T)^2$. An analogous estimate holds for $b : L^2(Q_T)^2 \to L^2(\Sigma)^2$. Thus, both reaction terms are Lipschitz continuous in $L^2(Q_T)^2$. Using the definition of F and the arguments leading to Equation (1.5) in the proof of Lemma 1.4.1, we obtain

$$\|F(y) - F(z)\|_{L^2(0,T;H^1(\Omega)^*)^2}^2 \leq 3 \left(\|d(y) - d(z)\|_{Q_T^2}^2 + \|b(y) - b(z)\|_{\Sigma^2}^2 c_\tau^2 + 2\lambda \|y_2 - z_2\|_{Q_T^2}^2 \right).$$

Thus, the Lipschitz continuity of d and b implies the continuity of F.

Boundedness. The boundedness condition (3.1) is due to Proposition 4.2.3 in combination with Equation (1.5) in the proof of Lemma 1.4.1. We conclude for the first component of F

$$\begin{aligned}\|F_1(y)\|^2_{L^2(0,T;H^1(\Omega)^*)} &\leq 2\left(\|d_1(y)+\lambda y_2\|^2_{L^2(Q_T)} + \|b_1(y)\|^2_{L^2(\Sigma)}c_\tau^2\right)\\ &= 2\int_0^T \left(\|G(y_1(t))\|^2_{L^2(\Omega_1)} + \|\bar{F}(y_1(t))\|^2_{L^2(\Omega_2)} + \|b_1(y(t))\|^2_{L^2(\Gamma)}c_\tau^2\right) dt\\ &\leq 2TM^2_{GEF}(2+c_\tau^2)\end{aligned}$$

for all $y \in Y = L^2(Q_T)^2$. Regarding the second component, we estimate similarly

$$\|F_2(y)\|^2_{L^2(0,T;H^1(\Omega)^*)} \leq 2\|d_2(y)-\lambda y_2\|^2_{L^2(Q_T)} = 2\int_0^T \nu^2\|G(y_1(t))\|^2_{L^2(\Omega_1)}dt \leq 2TM^2_{GEF}\nu^2.$$

The choice of ν implies $\nu^2 \leq 2 + c_\tau^2$. Therefore, the boundedness condition (3.1) holds with $M_{rea} := \sqrt{2T(2+c_\tau^2)}M_{GEF}$.

Conservation of mass. We state in Result 4.2.2 that the reaction terms (d_1, d_2) and b as well as the right-hand sides of the *PO_4-DOP* model fulfill the conservation of mass condition given in Remark 1.5.4. The same is true for the reaction terms $(d_1 + \lambda Id, d_2 - \lambda Id)$ and b because $d_1 + \lambda Id + d_2 - \lambda Id = d_1 + d_2$. Remark 1.5.4 states that the conservation of mass condition for $(d_1 + \lambda Id, d_2 - \lambda Id)$ and b is equivalent to the desired condition (3.2) for the operator F.

4.4.3 Stationary solutions of the PO_4-DOP model

Let $C \in \mathbb{R}$. In this section, we verify the assumptions of Theorem 3.3.2 by modifying the arguments of Section 4.4.2. Theorem 3.3.2 provides a stationary solution with the constant mass C of the time-independent *PO_4-DOP* model.

First, we introduce the time-independent *PO_4-DOP* model. Let $\Lambda = L^2(\Omega)^2$. The right-hand side is $f_{stat} = 0 \in (H^1(\Omega)^*)^2$. The operator $F_{stat} : \Lambda \to (H^1(\Omega)^*)^2$ is defined by a time-independent version of the *PO_4-DOP* model's reaction terms. Since their dependence on time originates from the continuous insolation function I, we fix I in some point of time, for example, in $t = 0$. The results of Section 4.2.2 guarantee that $G(0) : L^2(\Omega) \to L^2(\Omega)$ is well-defined. The same is true for $E(0)$ and $\bar{F}(0)$ and therefore also for $d(0) : \Lambda \to L^2(\Omega)^2$ and $b(0) : \Lambda \to L^2(\Gamma)^2$. Thus, we can define F_{stat} by means of $(d_1(0) + \lambda Id_{L^2(\Omega)}, d_2(0) - \lambda Id_{L^2(\Omega)})$ according to Lemma 1.4.1.

All arguments used to prove continuity, boundedness, and conservation of mass in the periodic case are either valid for almost all $t \in [0, T]$ (Lipschitz continuity in Section 4.4.1, Proposition 4.2.3, conservation of mass condition in Result 4.2.2) or have a time-independent equivalent (Equation (1.5) in the proof of Lemma 1.4.1). In particular, these properties hold for $t = 0$ because of the continuity of I. Therefore, continuity, boundedness, and conservation of mass can be proved as in the periodic case, the only difference being the missing integrals with respect to time.

4.5 The fixed point iteration and uniqueness

This section addresses the fixed point iteration, a method that is used to compute periodic solutions of the PO_4-DOP model. In addition, we present the results of a numerical test concerning uniqueness of periodic solutions.

4.5.1 The fixed point iteration

According to Section 4.4.1, a transient solution of the PO_4-DOP model associated with a known initial value is unique. Therefore, a periodic solution is uniquely determined by its initial (and terminal) value. To describe the initial value as a fixed point, we refer to the unique solution associated with the initial value $y_0 \in L^2(\Omega)^2$ as $y \in W(0,T)^2$. Then, the operator

$$A : L^2(\Omega)^2 \to L^2(\Omega)^2, \quad y_0 \mapsto y(T)$$

maps the initial to the terminal value of y. The expression $y(T)$ is an abridged form of $(E_T \circ E_C^2)(y)$. The insertion operator E_T is defined in the proof of Lemma 2.2.3, and E_C^2 is the continuous embedding of $W(0,T)^2$ in $C([0,T]; L^2(\Omega))^2$ (cf. Theorem 1.1.2(1)). Both operators are linear and continuous. The uniqueness of the solution y ensures that A is well-defined.

Obviously, an element $\bar{y}_0 \in L^2(\Omega)^2$ is the initial value of a periodic solution if and only if it is a fixed point of A. According to Remark VI.1.9 of Gajewski et al. [7], A is contractive if the operators in the model equation, B^2 and F, fulfill a variant of strict monotonicity. In this case, Banach's Fixed Point Theorem yields a unique fixed point $\bar{y}_0 \in L^2(\Omega)^2$ and therefore a unique periodic solution. In addition, the fixed point is equal to the limit of the iteratively defined sequence $(x_n)_{n\in\mathbb{N}}$, given by

$$x_0 := y_0 \in L^2(\Omega)^2 \quad \text{and} \quad x_n = A(x_{n-1}) \quad \text{for all } n \in \mathbb{N} \setminus \{0\}. \tag{4.5}$$

The starting value x_0 is an arbitrary element of $L^2(\Omega)^2$. The n-th member is the terminal value of the transient solution associated with the initial value x_{n-1}.

The fixed point iteration approximates a periodic solution by computing the sequence (4.5) iteratively. The iteration stops as soon as the difference between two successive members, i.e., between the initial value x_n and the terminal value x_{n+1} of a transient solution, is sufficiently small. In this case, the transient solution corresponding to the initial value x_n approximates a periodic solution. Banach's Fixed Point Theorem provides information about the quality of approximation in the form of error estimates.

In the context of ecosystem models, the fixed point iteration is often called spin-up. Periodic solutions are considered as an equilibrium that is reached after a sufficient number of years (= iterations).

The PO_4-DOP model's reaction terms do not fulfill the variant of strict monotonicity required for the convergence of the sequence (4.5). Parts of the reaction terms are not even monotone, for example, the integral with respect to x_3 in E and the summand $-\lambda y_2$ in the equation for y_1. The absence of the variant of strict monotonicity is in accordance with Theorem 3.2.1. This theorem provides several periodic solutions distinguished by mass. If the reaction terms were strictly monotone, however, Banach's Fixed Point Theorem would yield a unique fixed point of A and therefore a unique periodic solution.

Despite the missing mathematical justification, the fixed point iteration is frequently used to compute periodic solutions of the PO_4-DOP model, for example, by Prieß et al. [17, Section 2.4] or Parekh et al. [15, Section 3]. After a large number of iterations (3000 or 3500 years in the examples), the method actually yields an approximation of a periodic solution.

The fixed point iteration is considered feasible if all starting values with the fixed mass $C \in \mathbb{R}$ yield the same periodic solution. Because of the uncertainty with regard to convergence, analytical results about feasibility cannot be expected. For this reason, we approach the question of feasibility by means of a numerical test, using a two-dimensional version of the PO_4-DOP model.

We describe the implementation of the fixed point iteration for the two-dimensional version of the PO_4-DOP model in the next section. Afterwards, we explain the test in detail and give the results.

4.5.2 Implementation

The fixed point iteration for the two-dimensional PO_4-DOP model is built on the software NaSt2D by Griebel et al. [8] which is available on the homepage[1] of the authors. Since the program is described in detail in the cited book, we provide only the main features and concentrate on our adaptions.

Written in the C programming language, the original program is designed to solve the Navier-Stokes equations for incompressible fluids on a quadratic domain in a finite time interval. Beside the equations for the two velocity components and pressure, the program considers an advection-diffusion equation modeling the influence of temperature. The equations for velocity, pressure, and temperature are iteratively solved via the Euler method. In one time step, each quantity is described by a matrix whose dimension corresponds to the discretization of the quadratic domain.

The original program covers different types of problems. We exclusively regard the case of driven cavity flow. This flow originates from a forcing at the upper side of the quadratic domain, such as a ribbon that is pulled over the surface or wind blowing in one direction. The

[1] `http://wissrech.ins.uni-bonn.de/research/projects/NaSt2D/index.html`. Retrieved February 1, 2016

forcing is modeled by a boundary condition. An input file, adapted to the problem of driven cavity flow, gives the opportunity to specify many influencing factors for the iteration, such as the size and structure of the domain, constants (e.g. Reynolds number), initial values, and boundary conditions for velocity. For the sake of comparability, we use a fixed input file in all test runs. In particular, the finite time interval on which the solution is computed is specified as $[0, 10]$. Furthermore, the quadratic domain is discretized by a grid of 50×50 quadratic cells.

We proceed with a list of our changes and additions to the original program.

- The equation for temperature is eliminated. The values for temperature remain constant throughout the iteration.
- Two additional advection-diffusion-reaction equations describe the concentrations of PO_4 and DOP. The discretization of advection is taken directly from the equation for temperature; the discretization of diffusion is additionally enhanced by a constant diffusion matrix. The reaction terms of the PO_4-DOP model are added to the equations. The depth of the upper (euphotic) layer is set to $\bar{h}_e = 0.4$, the total depth being $h_{\max} = 1$.
- The values for the PO_4-DOP model's parameters are taken from Kriest et al. [10].
- The constant boundary condition for driven cavity flow is replaced by the time-dependent function $bd(t) = (0.2t - 1)|0.2t - 1| - 0.2t + 1$ on the time interval $[0, 10]$. Because of $bd(0) = 0 = bd(10)$, the function can be extended periodically to $\mathbb{R}^+$. Figure 4.5.1 shows bd and a part of the extension.

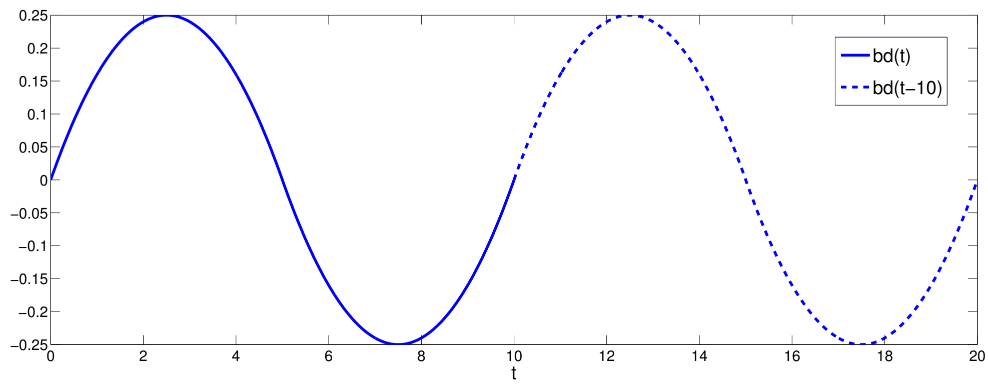

Figure 4.5.1: The function bd on $[0, 10]$ (solid line) and the periodic extension on $[10, 20]$ (dashed line).

The choice of bd guarantees a periodic forcing in the fixed point iteration.

- The fixed point iteration is implemented by means of a while loop. In each step, a transient solution on $[0, 10]$ with a suitable initial value is computed. The important features of the iteration are described below.

– The starting values, i.e., the initial values of PO_4 and DOP in the first step, are matrices of random numbers. The multiplication with a suitable factor ensures that their mass is equal to $C := 2.17$. To compute the mass, we implement the trapezoidal rule as an auxiliary function. The starting values of the velocity components and pressure are zero.

– In all other steps, the initial values for velocity, pressure, PO_4, and DOP are equal to the terminal values of the previous step. The terminal values are stored in a special file after each step and imported again when they are needed.

– After the transient solution is computed, we determine the difference between initial and terminal value of each quantity (velocity, pressure, PO_4, and DOP). The sum of the differences' 2-norms defines the residual `res`. We use the unweighted 2-norm since the two-dimensional domain is divided into cells of the same size.

– The while loop continues until `res` lies beneath a specified limit of tolerance c. We run the program with different values for c.

– During an additional time step following the while loop, the values of PO_4 and DOP at $t = 0$, $t = 2.5$, $t = 5$, and $t = 7.5$ are stored in an output file.

The described fixed point iteration computes periodic solutions for PO_4 and DOP as well as for velocity and pressure. This kind of computation, called "online" mode, is applied by Parekh et al. [15, Section 2.1] as well. The alternative "offline" mode requires a given velocity which is equal throughout the iteration. Prieß et al. [17], for instance, use special matrices to approximate both velocity and the diffusion coefficient. Because of the prescribed velocity $\mathbf{v}$, the method (4.5) is a continuous version of an "offline" computation. We indicate in the next section why the fixed point iteration described above nevertheless approximates (4.5).

The fixed point iteration can be easily adapted to stationary solutions (cf. Section 3.3). Since the boundary condition bd is responsible for the solution's periodicity, it suffices to replace bd by a constant value.

4.5.3 Numerical test

As explained above, the fixed point iteration is considered feasible if all solutions computed with starting values with the same mass C are equal. To investigate feasibility, we run the fixed point iteration using four random starting values with the mass $C = 2.17$. Afterwards, we compare the four periodic solutions for PO_4 and DOP. We perform this test twice using the limit of tolerance $c = 10^{-4}$ and $c = 10^{-5}$, respectively.

In all of the eight test runs, the final residuals of the two velocity components and pressure are approximately 10^{-13}, 10^{-16}, and 10^{-11}, respectively. This implies that the change of velocity and pressure is negligible compared to the change of PO_4 and DOP in the last steps of the iteration. In this sense, the "online" fixed point iteration can be regarded as a numerical version of the "offline" method (4.5).

Before we proceed with the results concerning PO_4 and DOP, we clarify when two solutions are considered equal in the numerical context. Regarding one test consisting of four runs, we refer to the solution obtained in the i-th run as $(PO_4(i), DOP(i))$ for each $i \in \{1, \dots, 4\}$. The solutions $(PO_4(i), DOP(i))$ and $(PO_4(j), DOP(j))$ for $i, j \in \{1, \dots, 4\}$ are considered equal if their residual, i.e., the sum of $\|PO_4(i) - PO_4(j)\|$ and $\|DOP(i) - DOP(j)\|$ with $\|.\|$ denoting the discrete $C([0,T]; L^2(\Omega))$-norm, falls below c. Since the contribution of velocity and pressure to the total residual `res` is negligible, this definition is in accordance with the stopping criterion in the fixed point iteration.

We explain the discrete $C([0,T]; L^2(\Omega))$-norm using $PO_4(1) - PO_4(2)$ as an example. According to the definition of the algorithm in Section 4.5.2, the solutions $PO_4(1)$ and $PO_4(2)$ on $[0, 10]$ are represented by vectors of values at $t = 0$, $t = 2.5$, $t = 5$, and $t = 7.5$. The entries of $PO_4(1)$, for instance, are displayed in Figure 4.5.2. To measure $PO_4(1) - PO_4(2)$ in the desired norm, we subtract each entry of $PO_4(2)$ from the corresponding entry of $PO_4(1)$ and compute the 2-norm of the resulting matrices. The maximum of these four numbers corresponds to the discrete $C([0,T]; L^2(\Omega))$-norm of $PO_4(1) - PO_4(2)$.

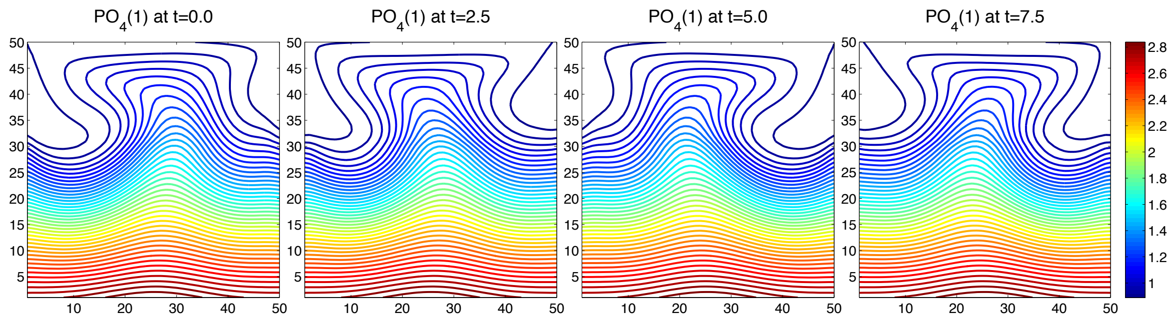

Figure 4.5.2: Contour lines of the entries of PO_4, obtained in the first run of Test 1. The axes show the discretization of the quadratic domain (50×50 cells).

The results of the two tests are presented in the Tables 4.5.1 and 4.5.2 on page 74. The four rows of each table correspond to the test runs. The first column indicates the number of steps required to reach the respective limit of tolerance. For all $i \in \{1, 2, 3\}$, the i-th of the remaining columns is divided into three subcolumns each of which has four entries. The j-th entry of the i-th column contains $\|PO_4(i) - PO_4(j)\|$ in the first and $\|DOP(i) - DOP(j)\|$ in the second subcolumn. The third subcolumn includes the residual between $(PO_4(i), DOP(i))$ and $(PO_4(j), DOP(j))$, i.e., the sum of the entries of the first two subcolumns. To avoid double entries, we consider only the residuals associated with the indices $j \in \{i, \dots, 4\}$ in the i-th column. Accordingly, a potential fourth column "Difference to Run 4" would contain only empty cells and zeros. Therefore, it is omitted.

We proceed with an interpretation of the results. Regarding the number of steps, we observe that all associated test runs have a similar length irrespective of the starting value. In particular, the fixed point iteration actually reaches a solution of the desired accuracy in all test runs. Thus, there is no indication that some starting values are better suited than others or that the fixed point iteration does not converge at all.

We compare the solutions by regarding the residuals listed in the third subcolumns. In the first test ($c = 10^{-4}$), the residuals range between $1.3 \cdot 10^{-5}$ and $9.5 \cdot 10^{-5}$. In the second test ($c = 10^{-5}$), the residuals range between $1.5 \cdot 10^{-6}$ and $5.8 \cdot 10^{-6}$. Thus, in both tests, all residuals lie beneath the corresponding limit of tolerance. This implies that all solutions are equal in the sense of the definition above.

In summary, the test provides no indication that the fixed point iteration might be infeasible.

Table 4.5.1: Residuals between all solutions of Test 1 ($c = 10^{-4}$). The norms of the differences are rounded to six decimal places and divided by 10^{-5}.

		Difference to Run 1			**Difference to Run 2**			**Difference to Run 3**		
Run	**Steps**	PO_4	DOP	Res.	PO_4	DOP	Res.	PO_4	DOP	Res.
1	356	0	0	0	-	-	-	-	-	-
2	357	4.4	3.6	8.0	0	0	0	-	-	-
3	355	0.9	0.4	1.3	4.5	4.0	9.5	0	0	0
4	357	1.7	0.9	2.6	3.2	2.7	5.9	1.5	1.4	2.9

Table 4.5.2: Residuals between all solutions of Test 2 ($c = 10^{-5}$). The norms of the differences are rounded to seven decimal places and divided by 10^{-6}.

		Difference to Run 1			**Difference to Run 2**			**Difference to Run 3**		
Run	**Steps**	PO_4	DOP	Res.	PO_4	DOP	Res.	PO_4	DOP	Res.
1	441	0	0	0	-	-	-	-	-	-
2	441	1.0	0.5	1.5	0	0	0	-	-	-
3	440	3.2	2.6	5.8	2.6	2.1	4.7	0	0	0
4	440	3.0	2.2	5.2	2.4	1.7	4.1	1.4	0.4	1.8

Chapter 5

Parameter identification in a marine ecosystem model

In this chapter, we consider the reaction terms' dependence on parameters. Model validation can be effected by adjusting the parameters in such a way that the model reproduces observational data "optimally" in some sense (cf. Fennel and Neumann [6, Section 1.1]). The process of finding "optimal" parameters is called parameter identification.

In the first subsection, we introduce parameter identification as an optimization problem and define optimal parameters. Furthermore, we prove the existence of optimal parameters under certain assumptions and give examples for reaction terms that are in accordance with these assumptions. Sections 5.2 and 5.3 are concerned with first and second order conditions for optimal parameters.

5.1 Existence of optimal parameters

We start with a hypothesis providing all important assumptions.

Hypothesis 5.1.1. *In addition to Hypothesis 1.2.1, we assume that the set of admissible parameters $U_{ad} \subseteq V$ is nonempty, closed, bounded, and convex. Let the data $y_d \in L^2(Q_T)^s$ and $u_d \in U_{ad}$ be given. Let furthermore $\gamma \geq 0$ and $y_0 \in L^2(\Omega)^s$. We abbreviate the initial value condition by $A(y) \in \{y(0) - y_0, y(0) - y(T)\}$ for all $y \in W(0,T)^s$.*

Remark 5.1.2. *In the context of parameter identification, the admissible set U_{ad} is often defined by box constraints. For each $i \in \{1, \ldots, n_p\}$, these are given by the bounds $u_{a,i}, u_{b,i} \in L^\infty(Q_T)$ or $L^\infty(\Sigma)$ depending on the character of U_i with $u_{a,i} \leq u_{b,i}$ almost everywhere. Then, $u \in U_{ad}$ if and only if $u \in V$ and*

$$u_{a,i}(x,t) \leq u_i(x,t) \leq u_{b,i}(x,t) \quad \text{for all } i \in \{1, \ldots, n_p\} \text{ and almost all } (x,t) \in Q_T \text{ or } \Sigma.$$

Clearly, the set U_{ad} defined in this way is a nonempty, closed, bounded, and convex subset of V.

We formulate the parameter identification problem for the general operator equation (1.6), extended by the reaction terms' dependence on the parameters, i.e., for

$$y' + B^s(y) + F(u, y) = f(u) \quad \text{in } L^2(0, T; H^1(\Omega)^*)^s \tag{5.1}$$

with $F : V \times Y \to L^2(0, T; H^1(\Omega)^*)^s$ and $f : V \to L^2(0, T; H^1(\Omega)^*)^s$.

First of all, we introduce and explain the components of the optimization problem associated with parameter identification.

1. In the context of parameter identification, we minimize the difference between model output and data y_d as well as the difference between parameter and target parameter u_d. Therefore, the associated optimization problem includes the least-squares cost function

   $$J : U \times L^2(Q_T)^s \to \mathbb{R}, \quad J(u, y) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2}\|u - u_d\|^2_U.$$

   The coefficient γ controls the influence of the last summand on the minimum. Target parameters u_d corresponding to real observational data y_d are seldom available. In this case, γ is set to zero, and the second summand of the cost function vanishes.

2. The optimization problem additionally features side conditions for y and u. The first side condition guarantees that y equals the model output corresponding to u. This condition is formulated by means of the operator $e : V \times W(0, T)^s \to L^2(0, T; H^1(\Omega)^*)^s$, defined by

   $$e(u, y) := y' + B^s(y) + F(u, y) - f(u) \quad \text{for all } (u, y) \in V \times W(0, T)^s.$$

   In addition, the initial value condition $A(y) = 0$ specifies if transient or periodic solutions are considered. The second side condition ensures that u belongs to U_{ad}.

Combining these components, we obtain the optimization problem

$$\begin{aligned} &\min J(u, y) \\ \text{subject to} \quad &e(u, y) = 0, \quad A(y) = 0, \quad u \in U_{ad}. \end{aligned}$$

To formulate the optimization problem without explicitly stating the side conditions, we define the set of all admissible pairs, i.e., all pairs that agree with the side conditions,

$$X_{ad} := \{(u, y) \in U_{ad} \times W(0, T)^s : e(u, y) = 0 \text{ and } A(y) = 0\} \subseteq U \times L^2(Q_T)^s.$$

Using this definition, the optimization problem can be written as

$$\min_{(u,y)\in X_{ad}} J(u, y). \tag{5.2}$$

Optimal parameters are defined by means of this optimization problem.

Definition 5.1.3. *The parameter $\bar{u} \in U_{ad}$ is called optimal for* (5.1) *and* (u_d, y_d) *if there exists a state $\bar{y} \in W(0,T)^s$ in such a way that the pair $(\bar{u}, \bar{y})$ belongs to X_{ad} and solves the minimization problem* (5.2)*, i.e.,*

$$J(\bar{u}, \bar{y}) \leq J(u, y) \quad \textit{for all } (u, y) \in X_{ad}.$$

The following existence theorem about optimal parameters covers the general case of parameters depending on space and time. Variable parameters are appropriate in some situations. Oschlies [13, Section 4], for instance, uses a variable growth rate to model fertilization with iron. The authors of the *PO_4-DOP-Fe* model state that one of their parameters "is unlikely to be uniform in space and time" (Parekh et al. [15, Section 2.3]). However, most parameters in marine ecosystem models are assumed to be constant. To account for that, we provide a corollary adapted to models with constant parameters in addition to the theorem.

Hinze et al. [9, Section 1.5.2] prove a similar existence result under the assumption that the model equation is uniquely solvable. We adapt their proof in such a way that the assumption of unique solvability can be dispensed with. The generalization is important for the periodic *PO_4-DOP* model which is not uniquely solvable.

Theorem 5.1.4. *In addition to Hypothesis 5.1.1, let the Banach space U be reflexive and $F : V \times Y \to L^2(0,T;H^1(\Omega)^*)^s$ and $f : V \to L^2(0,T;H^1(\Omega)^*)^s$ be weakly sequentially continuous. We assume that for every $u \in U_{ad}$ there exists $y \in W(0,T)^s$ such that $(u, y) \in X_{ad}$. Furthermore, let the set of admissible states $Y_{ad} := \{y \in W(0,T)^s : \exists u \in U_{ad} : (u, y) \in X_{ad}\}$ be bounded in $W(0,T)^s$ by a constant M_{ad}. Hence, there is an optimal parameter $\bar{u} \in U_{ad}$ for* (5.1) *and* (u_d, y_d).

Proof. Since the set $J(X_{ad})$ is bounded from below by zero, the infimum $j := \inf J(X_{ad})$ is finite. By definition of the infimum, there is a sequence $((u_n, y_n))_n \subseteq X_{ad}$ with $J(u_n, y_n) \to j$. Being an element of X_{ad}, the pair (u_n, y_n) satisfies

$$\left.\begin{array}{rcl} y_n' + B^s(y_n) + F(u_n, y_n) - f(u_n) = e(u_n, y_n) & = & 0 \\ A(y_n) & = & 0 \end{array}\right\} \text{ for all } n \in \mathbb{N}.$$

Since U_{ad} is bounded in U, so is the sequence $(u_n)_n$. Furthermore, y_n belongs to Y_{ad} which is assumed to be bounded by M_{ad}. Thus, the sequence $((u_n, y_n))_n$ is bounded in $U \times W(0,T)^s$.

Since U is assumed to be reflexive, so is $U \times W(0,T)^s$. Thus, we obtain a subsequence, denoted by $((u_n, y_n))_n$ as well, and a pair $(\bar{u}, \bar{y}) \in U \times W(0,T)^s$ with $(u_n, y_n) \rightharpoonup (\bar{u}, \bar{y})$.

We will prove that $\bar{u}$ is an optimal parameter according to Definition 5.1.3, i.e., that $(\bar{u}, \bar{y})$ belongs to X_{ad} and minimizes J on X_{ad}. To verify the first property, we use that the closed and convex set U_{ad} is weakly sequentially closed. This is a consequence from the Theorem of Mazur (see Yosida [27, Theorem V.1.2]). Thus, $u_n \rightharpoonup \bar{u}$ and $(u_n)_n \subseteq U_{ad}$ imply $\bar{u} \in U_{ad}$. Thus, $(\bar{u}, \bar{y})$ belongs to X_{ad} if $A(\bar{y}) = 0$ and $e(\bar{u}, \bar{y}) = 0$.

Using the notation of the proof of Lemma 2.2.3, we can define the initial value condition more precisely as $A(y_n) = E_0 \circ E_C^s(y_n) - y_0$ or $A(y_n) = E_0 \circ E_C^s(y_n) - E_T \circ E_C^s(y_n)$. Here, E_C^s is the continuous embedding of $W(0,T)^s$ in $C([0,T]; L^2(\Omega))^s$ (cf. Theorem 1.1.2(1)). We have proved before that the operators E_T and $E_0 : C([0,T]; L^2(\Omega))^s \to L^2(\Omega)^s$ are weakly sequentially continuous. The same is true for the linear and bounded operator E_C^s. Thus, the weak convergence of $(y_n)_n$ in $W(0,T)^s$ implies $A(y_n) \rightharpoonup A(\bar{y})$ for both versions of A. Since $A(y_n) = 0$ for all $n \in \mathbb{N}$, and the weak limit is unique, we arrive at $A(\bar{y}) = 0$.

Because of the continuous embedding of $W(0,T)^s$ in Y, the sequence $(y_n)_n$ converges weakly to $\bar{y}$ in Y. In particular, $(u_n, y_n) \rightharpoonup (\bar{u}, \bar{y})$ in $U \times Y$. The weak sequential continuity of F and f yields $F(u_n, y_n) \rightharpoonup F(\bar{u}, \bar{y})$ and $f(u_n) \rightharpoonup f(\bar{u})$ in $L^2(0,T; H^1(\Omega)^*)^s$. Additionally regarding the weak convergence of $(y_n)_n$ to $\bar{y}$ in $W(0,T)^s$, we conclude $e(u_n, y_n) \rightharpoonup e(\bar{u}, \bar{y})$. As in the last paragraph, the fact $e(u_n, y_n) = 0$ for all $n \in \mathbb{N}$ implies $e(\bar{u}, \bar{y}) = 0$.

At last, we show that $(\bar{u}, \bar{y})$ minimizes J on X_{ad}. Since $W(0,T)^s$ is continuously embedded in $L^2(Q_T)^s$, the sequence $(y_n)_n$ converges weakly to $\bar{y}$ in $L^2(Q_T)^s$ as well. Using the definitions of j and J as well as Theorem V.1.1(ii) of Yosida [27], applied to both sequences $(y_n - y_d)_n$ and $(u_n - u_d)_n$, we estimate

$$
\begin{aligned}
j = \lim_{n\to\infty} J(u_n, y_n) &= \liminf_{n\to\infty} \left(\frac{1}{2} \|y_n - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2} \|u_n - u_d\|^2_U \right) \\
&\geq \frac{1}{2} \|\bar{y} - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2} \|\bar{u} - u_d\|^2_U = J(\bar{u}, \bar{y}) \geq j.
\end{aligned}
$$

The last estimate $J(\bar{u}, \bar{y}) \geq j$ holds because $(\bar{u}, \bar{y}) \in X_{ad}$ and j is the infimum of $J(X_{ad})$. We conclude that $j = J(\bar{u}, \bar{y})$ is a minimum of $J(X_{ad})$. By definition, $\bar{u} \in U_{ad}$ is an optimal parameter for (5.1) and (u_d, y_d). □

In the following corollary, we consider spaces U and Y with special properties. The last two statements concern the case of constant parameters.

Corollary 5.1.5. *Theorem 5.1.4 remains valid if the weak sequential continuity of $F : V \times Y \to L^2(0,T; H^1(\Omega)^*)^s$ and $f : V \to L^2(0,T; H^1(\Omega)^*)^s$ is replaced by one of the following alternative assumptions.*

1. *The space $W(0,T)^s$ is compactly embedded in Y; F is weakly sequentially continuous with respect to the first component and demicontinuous with respect to the second, i.e., $F(u_n, y_n) \rightharpoonup F(u, y)$ for all $(u_n)_n \subseteq V$ with $u_n \rightharpoonup u$ in U and all $(y_n)_n \subseteq Y$ with $y_n \to y$ in Y. The functional f is weakly sequentially continuous.*

2. *The parameter space U is finite-dimensional; F is demicontinuous with respect to the first component and weakly sequentially continuous with respect to the second component, i.e., $F(u_n, y_n) \rightharpoonup F(u, y)$ for all $(u_n)_n \subseteq V$ with $u_n \to u$ in U and all $(y_n)_n \subseteq Y$ with $y_n \rightharpoonup y$ in Y. The functional f is demicontinuous.*

3. *The space $W(0,T)^s$ is compactly embedded in Y, U is finite-dimensional, and F and f are demicontinuous.*

Proof. In the proof of Theorem 5.1.4, the weak sequential continuity of F and f is used to conclude $F(u_n, y_n) \rightharpoonup F(\bar{u}, \bar{y})$ and $f(u_n) \rightharpoonup f(\bar{u})$. Clearly, the proof remains valid if $F(u_{n_k}, y_{n_k}) \rightharpoonup F(\bar{u}, \bar{y})$ and $f(u_{n_k}) \rightharpoonup f(\bar{u})$ hold for a subsequence of $((u_n, y_n))_n$. We prove the existence of such a subsequence under each of the corollary's three assumptions.

First, we regard the case that $W(0,T)^s$ is compactly embedded in Y. Converging weakly in $W(0,T)^s$, the sequence $(y_n)_n$ is bounded in this space. The compact embedding ensures that a subsequence $(y_{n_k})_k$ converges strongly in Y. Because of the uniqueness of the weak limit, the strong limit is equal to $\bar{y}$. The assumptions yield the desired convergence result.

Second, we consider a finite-dimensional parameter space U. Here, weak and strong convergence coincide, and the sequence $(u_n)_n$ thus converges strongly to $\bar{u}$. The desired convergence result follows from the assumptions about F and f.

In the final case, the considerations above are combined. Because of the finite dimension of U, the sequence $(u_n)_n$ converges strongly to $\bar{u}$. As in the first case, a subsequence $(y_{n_k})_k$ of $(y_n)_n$ converges strongly to $\bar{y}$ in Y because of the assumed compact embedding. The strong convergence of $((u_{n_k}, y_{n_k}))_k$ to $(\bar{u}, \bar{y})$ in $U \times Y$ and the assumed demicontinuity of F and f imply the desired convergence result. □

In the following subsection, we present two typical reaction terms which are in accordance with Corollary 5.1.5.

5.1.1 Examples

Linear growth. Choose $2 < p < \infty$ and $1 < q < \infty$ in such a way that $\frac{2}{p} + \frac{2}{q} = 1$ holds and that $W(0,T)$ is compactly embedded in $Y := L^q(Q_T)$ for all dimensions $n_d \in \{1,2,3\}$. A possible choice is $p = 6$ and $q = 3$ (cf. Růžička [19, Corollary 3.98]). The parameter space $U = V = L^p(Q_T)$ is reflexive because of the choice of p. Let $U_{ad} \subseteq U$ be a nonempty, closed, bounded, and convex set. Consider the reaction term

$$d : L^p(Q_T) \times L^q(Q_T) \to L^2(Q_T), \quad d(a,y)(x,t) = a(x,t)y(x,t).$$

For a fixed $a \in L^p(Q_T)$, the family consisting of the operators $d(t) : L^q(\Omega) \to L^2(\Omega)$ with $d(t)(v) = a(.,t)v$ for all $v \in L^q(\Omega)$ defines d in the sense of Hypothesis 1.2.1. Hölder's inequality with $p/2$ and $q/2$ ensures that d and $d(t)$ are well-defined. The spaces $\Lambda := L^q(\Omega)$ and $Y = L^q(Q_T)$ comply with (1.1). Thus, Hypothesis 1.2.1 is fulfilled.

We prove that d satisfies the assumption of Corollary 5.1.5(1). First, $W(0,T)$ is compactly embedded in $L^q(Q_T)$ by assumption. Furthermore, we have to prove that, given $a_n \rightharpoonup a$ in $L^p(Q_T)$, $y_n \to y$ in $L^q(Q_T)$, and $v \in L^2(0,T;H^1(\Omega))$, the operator F, defined by d in the sense of Lemma 1.4.1, fulfills

$$\langle F(a_n, y_n) - F(a,y), v\rangle_{L^2(0,T;H^1(\Omega)^*)} = \int_{Q_T} (a_n y_n - ay) v d(x,t) \to 0.$$

We investigate the convergence of both summands on the right-hand side of

$$\int_{Q_T} (a_n y_n - ay) v d(x,t) = \int_{Q_T} a_n (y_n - y) v d(x,t) + \int_{Q_T} (a_n - a) y v d(x,t) \tag{5.3}$$

separately. Preliminarily, we deduce

$$\frac{1}{q} = \frac{1}{2} - \frac{1}{p} = \frac{p-2}{2p} \tag{5.4}$$

from the assumption about p and q. To treat the first summand on the right-hand side of (5.3), we use Hölder's inequality twice, first with the exponent q and the Hölder conjugate

$$\left(1 - \frac{1}{q}\right)^{-1} = \left(1 - \frac{p-2}{2p}\right)^{-1} = \left(\frac{p+2}{2p}\right)^{-1} = \frac{2p}{p+2},$$

computed by means of (5.4), and second with $(p+2)/p$ and the Hölder conjugate

$$\left(1 - \frac{p}{p+2}\right)^{-1} = \left(\frac{p+2-p}{p+2}\right)^{-1} = \frac{p+2}{2}.$$

We obtain

$$\begin{aligned}
\int_{Q_T} a_n (y_n - y) v d(x,t) &\leq \left(\int_{Q_T} |a_n v|^{\frac{2p}{p+2}} d(x,t)\right)^{\frac{p+2}{2p}} \|y_n - y\|_{L^q(Q_T)} \\
&\leq \left[\left(\int_{Q_T} v^2 d(x,t)\right)^{\frac{p}{p+2}} \left(\int_{Q_T} |a_n|^p d(x,t)\right)^{\frac{2}{p+2}}\right]^{\frac{p+2}{2p}} \|y_n - y\|_{L^q(Q_T)} \\
&= \|v\|_{L^2(Q_T)} \|a_n\|_{L^p(Q_T)} \|y_n - y\|_{L^q(Q_T)}.
\end{aligned}$$

The first norm is finite because $L^2(0,T;H^1(\Omega))$ is continuously embedded in $L^2(Q_T)$. Furthermore, the sequence $(a_n)_n$ is weakly convergent and therefore bounded in $L^p(Q_T)$. Thus, the strong convergence of $(y_n)_n$ to y in $L^q(Q_T)$ ensures that the first summand on the right-hand side of (5.3) converges to zero.

Since $(a_n)_n$ converges weakly to a in $L^p(Q_T)$, the second summand on the right-hand side of (5.3) converges to zero if yv belongs to $L^{\frac{p}{p-1}}(Q_T)$ which is isomorphic to the dual space of $L^p(Q_T)$. We apply Hölder's inequality with $2(p-1)/(p-2)$ and the Hölder conjugate

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

and obtain using (5.4) twice

$$\|yv\|_{L^{\frac{p}{p-1}}(Q_T)}^{\frac{p}{p-1}} = \int_{Q_T} |yv|^{\frac{p}{p-1}} d(x,t) \leq \left(\int_{Q_T} |y|^q d(x,t)\right)^{\frac{p-2}{2(p-1)}} \left(\int_{Q_T} v^2 d(x,t)\right)^{\frac{p}{2(p-1)}}$$

$$= \left(\int_{Q_T} |y|^q d(x,t)\right)^{\frac{1}{q}\cdot\frac{q(p-2)}{2(p-1)}} \left(\int_{Q_T} v^2 d(x,t)\right)^{\frac{1}{2}\cdot\frac{p}{p-1}} = \left(\|y\|_{L^q(Q_T)}\|v\|_{L^2(Q_T)}\right)^{\frac{p}{p-1}}.$$

Because of the choice of y and v, the last expression is finite. Thus, yv belongs to $L^{\frac{p}{p-1}}(Q_T)$ which implies that the second summand on the right-hand side of (5.3) converges to zero.

A saturation function. Choose p and q as in the previous example and consider the reaction term

$$d : L^p(Q_T) \times \mathbb{R}_{>0} \times L^q(Q_T) \to L^2(Q_T), \quad d(\alpha, K, y)(x,t) = \alpha(x,t)\frac{y(x,t)}{|y(x,t)| + K}$$

featuring the parameter vector $u = (\alpha, K)$. The operator d models a reaction with a half saturation constant K and a variable maximum rate α. A reaction term of this kind, featuring a constant maximum rate, plays a central role in the *PO_4-DOP* model (cf. Section 4.2.2).

We set $U := L^p(Q_T) \times \mathbb{R}$, $V := L^p(Q_T) \times \mathbb{R}_{>0}$, and $Y := L^q(Q_T)$. The parameter space U is reflexive. For a fixed $(\alpha, K) \in V$, the family consisting of the operators $d(t)$: $L^q(\Omega) \to L^2(\Omega)$ with $d(t)(v) = \alpha(\,.\,,t)v/(|v| + K)$ for all $v \in L^q(\Omega)$ defines d in the sense of Hypothesis 1.2.1. The operators d and $d(t)$ are well-defined since the fraction is bounded by 1 according to Lemma 4.2.1, and $p > 2$ implies that $L^p(\Psi)$ is continuously embedded in $L^2(\Psi)$ for $\Psi \in \{\Omega, Q_T\}$. The spaces $\Lambda = L^q(\Omega)$ and $Y = L^q(Q_T)$ fulfill condition (1.1). Thus, Hypothesis 1.2.1 is satisfied. The set of admissible parameters is given by

$$U_{ad} := \{(\alpha, K) \in L^p(Q_T) \times \mathbb{R} : \alpha_a \leq \alpha \leq \alpha_b \text{ almost everywhere and } K_a \leq K \leq K_b\}$$

using the bounds $\alpha_a, \alpha_b \in L^\infty(Q_T)$ with $\alpha_a \leq \alpha_b$ almost everywhere and $K_a, K_b \in \mathbb{R}_{>0}$ with $K_a \leq K_b$. Obviously, $U_{ad} \subseteq V$.

We prove that d satisfies the assumption of Corollary 5.1.5(1). First, $W(0,T)$ is compactly embedded in $L^q(Q_T)$ by assumption. The proof of Theorem 5.1.4 reveals that it suffices to prove the second property of Corollary 5.1.5(1) for parameter sequences in U_{ad}. Thus, let $(\alpha_n, K_n), (\alpha, K) \in U_{ad}$ with $(\alpha_n, K_n) \rightharpoonup (\alpha, K)$ in U and $y_n \to y$ in $L^q(Q_T)$. Since the second parameter is real, K_n converges strongly to K. Let F be the operator defined by d in the sense of Lemma 1.4.1. We have to verify that

$$\begin{aligned}\langle F(\alpha_n, K_n, y_n) - F(\alpha, K, y), v\rangle_{L^2(0,T;H^1(\Omega)^*)} &= \int_{Q_T}\left(\alpha_n\frac{y_n}{|y_n| + K_n} - \alpha\frac{y}{|y| + K}\right) v\, d(x,t)\\ &= \int_{Q_T}(\alpha_n - \alpha)\frac{y_n}{|y_n| + K_n} v\, d(x,t) + \int_{Q_T}\alpha\left(\frac{y_n}{|y_n| + K_n} - \frac{y}{|y| + K}\right) v\, d(x,t) \quad (5.5)\end{aligned}$$

converges to zero for all $v \in L^2(0,T;H^1(\Omega))$.

Let $v \in L^2(0,T;H^1(\Omega))$. To begin with, we prove that $(y_n v)/(|y_n| + K_n) - (yv)/(|y| + K)$ converges strongly to zero in $L^{\frac{p}{p-1}}(Q_T)$. Given a fixed $(x,t) \in Q_T$, we obtain, omitting the argument (x,t) for the sake of shortness,

$$\left|\frac{y_n v}{|y_n|+K_n} - \frac{yv}{|y|+K}\right| \leq \left|\frac{y_n v}{|y_n|+K_n} - \frac{yv}{|y|+K_n}\right| + \left|\frac{yv}{|y|+K_n} - \frac{yv}{|y|+K}\right|$$
$$\leq \frac{|v|}{K_n}|y_n - y| + \max_{\tilde{K}\in[K_a,K_b]} \frac{|yv|}{(|y|+\tilde{K})^2}|K_n - K| \leq \frac{|v|}{K_a}\left(|y_n - y| + |K_n - K|\right).$$

In the second line, we use Lemma 4.2.1 to estimate the first summand and the mean value theorem to estimate the second. Both Lipschitz constants are bounded because of the box constraints. In particular, we estimate the second one by

$$\frac{|y||v|}{(|y|+\tilde{K})^2} \leq \frac{(|y|+\tilde{K})|v|}{(|y|+\tilde{K})^2} = \frac{|v|}{|y|+\tilde{K}} \leq \frac{|v|}{K_a}$$

using $|y| \geq 0$ and $\tilde{K} \geq K_a$.

We estimate the upper bound $|v|\,|y_n - y| + |v|\,|K_n - K|$ in $L^{\frac{p}{p-1}}(Q_T)$. Treating the norm of the first summand in the same way as yv in the last section, we conclude

$$\|v(y_n - y)\|^{\frac{p}{p-1}}_{L^{\frac{p}{p-1}}(Q_T)} \leq \left(\|v\|_{L^2(Q_T)}\|y_n - y\|_{L^q(Q_T)}\right)^{\frac{p}{p-1}}.$$

An analogous estimate holds for the second summand. Here, the constant function 1 takes on the role of $|y_n - y|$ after the constant expression $|K_n - K|$ has left the integral.

Combining the results, we arrive at

$$\left\|\frac{y_n v}{|y_n|+K_n} - \frac{yv}{|y|+K}\right\|_{L^{\frac{p}{p-1}}(Q_T)} \leq \frac{\|v\|_{L^2(Q_T)}}{K_a}\left(\|y_n - y\|_{L^q(Q_T)} + |Q_T|^{\frac{1}{q}}|K_n - K|\right).$$

The right-hand side converges to zero because v belongs to $L^2(Q_T)$ and the sequences $(y_n)_n$ and $(K_n)_n$ converge strongly to y and K, respectively.

Finally, we deal with the convergence of the two summands in (5.5) to zero. The sequence $\alpha_n - \alpha$ converges weakly to zero in $L^p(Q_T)$. In addition, $(y_n v)/(|y_n|+K_n)$ converges strongly in $L^{\frac{p}{p-1}}(Q_T)$ which is isomorphic to the dual space of $L^p(Q_T)$. Thus, the first summand in (5.5) converges to zero.

The second summand can be estimated using Hölder's inequality with the exponents p and $p/(p-1)$. The upper bound obtained in this way converges to zero since $\alpha \in L^p(Q_T)$, and the difference $(y_n v)/(|y_n|+K_n) - (yv)/(|y|+K)$ converges strongly in $L^{\frac{p}{p-1}}(Q_T)$ to zero.

Thus, the reaction term d fulfills all assumptions of Corollary 5.1.5(1).

5.2 Optimality conditions in the transient case

Optimality conditions provide a means to describe optimal parameters. In this section, we show that, given certain assumptions, optimality conditions for the parameter identification problem associated with a transient model equation exist. Because of Theorem 2.2.1, it is reasonable to assume that the transient model equation is uniquely solvable. On the basis of this assumption, we can formulate an equivalent of the parameter identification problem (5.2) depending on u instead of (u, y) (cf. Section 5.2.1). Section 5.2.2 is concerned with first and second order optimality conditions for this "reduced" optimization problem.

Let the following hypothesis be valid throughout this section.

Hypothesis 5.2.1. *In addition to Hypothesis 5.1.1 with $A(y) := y(0) - y_0$, we assume that U is a Hilbert space and that the equation* (5.1) *has a unique transient solution $y(u)$ for each parameter $u \in V$. Furthermore, let $F : V \times Y \to L^2(0,T;H^1(\Omega)^*)^s$ and $f : V \to L^2(0,T;H^1(\Omega)^*)^s$ be twice continuously Fréchet differentiable.*

Suppose that, for every $(\bar{u}, \bar{y}) \in V \times Y$, the operator $F'_y(\bar{u}, \bar{y}) : Y \to L^2(0,T;H^1(\Omega)^*)^s$ has a linear extension $\hat{F} : L^2(0,T;H^1(\Omega))^s \to L^2(0,T;H^1(\Omega)^*)^s$, characterized by

$$\hat{F}(\tilde{y}) = F'_y(\bar{u}, \bar{y})\tilde{y} \quad \text{for all } \tilde{y} \in Y.$$

The extension $\hat{F}$ is generated by a family $(\hat{F}(t))_t$, defined on $\Lambda = H^1(\Omega)^s$, and the operators $\hat{F}(t) : H^1(\Omega)^s \to (H^1(\Omega)^*)^s$ fulfill the Lipschitz condition

$$\|\hat{F}(t)(y(t)) - \hat{F}(t)(z(t))\|_{(H^1(\Omega)^*)^s} \leq L' \|y(t) - z(t)\|_{\Omega^s} \quad \text{for all } y, z \in L^2(0,T;H^1(\Omega))^s$$

with a Lipschitz constant $L' > 0$ independent of t.

5.2.1 Parameter-to-state map and reduced cost function

The following map connects a parameter with the corresponding solution of the equation (5.1). Hypothesis 5.2.1 ensures that the definition is meaningful.

Definition 5.2.2. *The map $S : V \to W(0,T)^s$, $u \mapsto y(u)$, is called parameter-to-state map.*

The next theorem treats the Fréchet differentiability of S. As a corollary, we obtain that transient solutions depend continuously on the parameters.

Theorem 5.2.3. *The parameter-to-state map $S : V \to W(0,T)^s$ is twice continuously Fréchet differentiable. For every $u \in V$, the derivative $S'(u) \in \mathcal{L}(U, W(0,T)^s)$ maps $v \in U$ to the solution $h := S'(u)v$ of the initial value problem*

$$\begin{aligned} h' + B^s(h) + F'_y(u, S(u))h &= f'(u)v - F'_u(u, S(u))v \\ h(0) &= 0. \end{aligned}$$

The second derivative $S''(u) \in \mathcal{L}(U, \mathcal{L}(U, W(0,T)^s))$ maps $v, w \in U$ to the solution $a :=$

$[S''(u)v]w$ *of the initial value problem*

$$\begin{aligned}a' + B^s(a) + F'_y(u,S(u))a = [f''(u)v]w - [F''_{yu}(u,S(u))v]S'(u)w - [F''_{yy}(u,S(u))S'(u)v]S'(u)w \\ - [F''_{uu}(u,S(u))v]w - [F''_{uy}(u,S(u))S'(u)v]w \\ a(0) = 0.\end{aligned}$$

Following Zeidler [28, Remark 4.6], we will henceforth omit the squared brackets separating the arguments of the second derivatives. Furthermore, two equal arguments are denoted by one squared argument. For instance, we use $S''(u)vw$ instead of $[S''(u)v]w$ and $S''(u)v^2$ instead of $S''(u)vv$.

Proof. First of all, we ensure that the initial value problems formulated in the theorem are uniquely solvable. Thanks to Hypothesis 5.2.1, the restriction $F_1 := F'_y(u,S(u))$ of $\hat{F}$ is generated by the family $(\hat{F}(t))_t$. The components $\hat{F}(t)$ fulfill the Lipschitz condition with a Lipschitz constant independent of t. Furthermore, $F'_y(u,S(u))$ is linear and therefore homogeneous. Linearity and (Lipschitz) continuity imply that $F'_y(u,S(u))$ is also weakly continuous. The right-hand sides of both equations belong to $L^2(0,T;H^1(\Omega)^*)^s$ by definition of F and f. Thus, Theorem 2.2.1 with $F_2 := 0$ yields a unique solution for each initial value problem. Both solutions belong to $W(0,T)^s$.

We employ the Implicit Function Theorem (cf. Zeidler [28, Theorem 4.B(d)]) to show that S is twice continuously Fréchet differentiable and to compute the derivatives.

Using the abbreviations $W := W(0,T)^s$ and $Z := L^2(0,T;H^1(\Omega)^*)^s$, we define

$$\Phi : V \times W \to Z \times L^2(\Omega)^s, \quad \Phi(u,y) := (y' + B^s(y) + F(u,y) - f(u), y(0) - y_0).$$

Let $\bar{u} \in V$ and $\bar{y} := S(\bar{u})$. The definition of S yields $\Phi(u,S(u)) = 0$ for all $u \in V$ and thus, in particular, $\Phi(\bar{u},\bar{y}) = 0$. It remains to be shown that Φ is twice continuously Fréchet differentiable, that the partial derivative Φ'_y is continuous at $(\bar{u},\bar{y})$, and that $\Phi'_y(\bar{u},\bar{y})$ is bijective.

Concerning the first property, we prove that all summands of Φ are twice continuously Fréchet differentiable at $(\bar{u},\bar{y})$.

The temporal derivative, the operator B^s, the insertion operator $E_0 : C([0,T];L^2(\Omega))^s \to L^2(\Omega)^s$ (see the proof of Lemma 2.2.3), and the continuous embedding $E^s_C : W(0,T)^s \to C([0,T];L^2(\Omega))^s$ are linear and bounded and thus twice continuously Fréchet differentiable. So are the constant y_0 and the right-hand side f. By assumption, the embedding $E_Y : W \to Y$ is continuous and linear, and $F : V \times Y \to Z$ is twice continuously Fréchet differentiable. Thus, the composition $F|_{V\times W} = F \circ (Id_U|_V, E_Y)$ is twice continuously Fréchet differentiable as well.

In summary, $\Phi : V \times W \to Z \times L^2(\Omega)^s$ is twice continuously Fréchet differentiable. All first and second partial derivatives exist and are continuous according to Zeidler [28, Proposition 4.14]. In particular, this is true for Φ'_y.

We proceed with the bijectivity of $\Phi'_y(\bar{u},\bar{y}) \in \mathcal{L}(W, Z \times L^2(\Omega)^s)$, given by

$$\Phi'_y(\bar{u},\bar{y})h = (h' + B^s(h) + F'_y(\bar{u},\bar{y})h, h(0)) \in Z \times L^2(\Omega)^s \quad \text{for every } h \in W.$$

To show that $\Phi'_y(\bar{u},\bar{y})$ is onto, let $(z, z_0) \in Z \times L^2(\Omega)^s$. The surjectivity of $\Phi'_y(\bar{u},\bar{y})$ is equivalent to the existence of an element $h \in W$ that fulfills the initial value problem

$$h' + B^s(h) + F'_y(\bar{u},\bar{y})h = z, \qquad h(0) = z_0. \tag{5.6}$$

At the beginning of this proof, we argued that an initial value problem with the "reaction term" $F'_y(\bar{u},\bar{y})$ is uniquely solvable in W. Therefore, $\Phi'_y(\bar{u},\bar{y})$ is onto.

Being linear, $\Phi'_y(\bar{u},\bar{y})$ is injective if and only if the kernel is trivial. An element h of the kernel is characterized by solving the initial value problem

$$h' + B^s(h) + F'_y(\bar{u},\bar{y})h = 0, \qquad h(0) = 0.$$

Again, the arguments above show that this problem has a unique solution which is obviously equal to the zero function. Thus, $h = 0$, and the operator $\Phi'_y(\bar{u},\bar{y})$ is injective.

As a result, $\Phi'_y(\bar{u},\bar{y})$ is bijective and has the inverse $\Phi'_y(\bar{u},\bar{y})^{-1} : Z \times L^2(\Omega)^s \to W$, mapping $(z, z_0) \in Z \times L^2(\Omega)^s$ to the solution h of the initial value problem (5.6).

The Implicit Function Theorem yields an open neighborhood $\tilde{V} \subseteq V$ of $\bar{u}$ and a twice continuously differentiable map $\tilde{S} : \tilde{V} \to Z \times L^2(\Omega)^s$ such that $\Phi(u, \tilde{S}(u)) = 0$ for all $u \in \tilde{V}$. However, this condition implies

$$\tilde{S}(u)' + B^s(\tilde{S}(u)) + F(u, \tilde{S}(u)) - f(u) = 0, \qquad \tilde{S}(u)(0) - y_0 = 0$$

and thus $S = \tilde{S}$ in the neighborhood $\tilde{V}$ according to Definition 5.2.2. As a consequence, S is twice continuously differentiable at every $u \in \tilde{V}$. Since $\bar{u}$ was chosen arbitrarily, this result can be extended to every $u \in V$.

The proof of the Implicit Function Theorem [28, Equation (23), p. 153] reveals that the derivative of $S'(\bar{u}) \in \mathcal{L}(U, W)$ is equal to

$$S'(\bar{u})v = -\Phi'_y(\bar{u},\bar{y})^{-1}(\Phi'_u(\bar{u},\bar{y})v) = \Phi'_y(\bar{u},\bar{y})^{-1}(-\Phi'_u(\bar{u},\bar{y})v) \quad \text{for all } v \in U.$$

We calculate that $\Phi'_u(\bar{u},\bar{y}) \in \mathcal{L}(U, Z \times L^2(\Omega)^s)$ is given by

$$\Phi'_u(\bar{u},\bar{y})v = (F'_u(\bar{u},\bar{y})v - f'(u)v, 0) \in Z \times L^2(\Omega)^s \quad \text{for all } v \in U.$$

The last identities in combination with Equation (5.6) yield the assertion of the theorem.

The proof of the Implicit Function Theorem [28, Equation (25), p. 154] also contains a formula for the second derivative $S''(\bar{u}) \in \mathcal{L}(U, \mathcal{L}(U, W))$. Provided that $v, w \in U$, this formula yields

$$\begin{aligned} S''(\bar u)vw &= \Phi'_y(\bar u,\bar y)^{-1}\left([-\Phi''_{yu}(\bar u,\bar y)v - \Phi''_{yy}(\bar u,\bar y)S'(\bar u)v]\Phi'_y(\bar u,\bar y)^{-1}[-\Phi'_u(\bar u,\bar y)w]\right) \\ &\quad + \Phi'_y(\bar u,\bar y)^{-1}\left([-\Phi''_{uu}(\bar u,\bar y)v - \Phi''_{uy}(\bar u,\bar y)S'(\bar u)v]w\right). \end{aligned} \tag{5.7}$$

To transform this expression, we compute the second partial derivatives of Φ. Given $v, w \in U$ and $y, z \in W$, these are equal to

$$\begin{aligned} \Phi''_{yy}(\bar u,\bar y)yz &= (F''_{yy}(\bar u,\bar y)yz, 0); \\ \Phi''_{uu}(\bar u,\bar y)vw &= (F''_{uu}(\bar u,\bar y)vw - f''(\bar u)vw, 0); \\ \Phi''_{yu}(\bar u,\bar y)vy &= (F''_{yu}(\bar u,\bar y)vy, 0); \\ \Phi''_{uy}(\bar u,\bar y)yv &= (F''_{uy}(\bar u,\bar y)yv, 0). \end{aligned}$$

Our previous results show that the object $\Phi'_y(\bar u,\bar y)^{-1}[-\Phi'_u(\bar u,\bar y)w]$ at the end of the first line of (5.7) equals $S'(\bar u)w$. Inserting the second derivatives of Φ into (5.7), we obtain

$$\begin{aligned} S''(\bar u)vw = \Phi'_y(\bar u,\bar y)^{-1}(&-F''_{yu}(\bar u,\bar y)vS'(\bar u)w - F''_{yy}(\bar u,\bar y)S'(\bar u)vS'(\bar u)w \\ &- (F''_{uu}(\bar u,\bar y)vw - f''(\bar u)vw) - F''_{uy}(\bar u,\bar y)S'(\bar u)vw, 0). \end{aligned}$$

This is equivalent to the theorem's last assertion. □

We use a variant of the parameter-to-state map S to eliminate the variable y in the cost function J.

Definition 5.2.4. *Let J be defined as in Section 5.1 and S as in Definition 5.2.2. We refer to the continuous embedding of $W(0,T)^s$ in $L^2(Q_T)^s$ as E^s_W.*

1. *The variant of the parameter-to-state map $\mathcal{S} := E^s_W \circ S : V \to L^2(Q_T)^s$ is called observation operator.*

2. *The function $J_{red} : V \to \mathbb{R}$, defined by $J_{red} = J \circ (Id_U|_V, \mathcal{S})$, i.e.,*

$$J_{red}(u) = \frac{1}{2}\|\mathcal{S}(u) - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2}\|u - u_d\|^2_U \quad \text{for every } u \in V,$$

is called reduced cost function.

The name "observation operator" is due to the fact that the range of $\mathcal{S}$ lies in the same space as the observation y_d.

Henceforth, we regard the minimization problem

$$\min_{u \in U_{ad}} J_{red}(u) \tag{5.8}$$

instead of (5.2). The following lemma ensures that (5.8) and (5.2) are equivalent.

Lemma 5.2.5. *The parameter $\bar{u} \in U_{ad}$ is optimal for* (5.1) *and* (u_d, y_d) *if and only if it solves the minimization problem* (5.8)*.*

Proof. Let $\bar{u} \in U_{ad}$. Definition 5.1.3 states that $\bar{u}$ is optimal for (5.1) and (u_d, y_d) if and only if there exists a state $\bar{y} \in W(0,T)^s$ in such a way that $(\bar{u}, \bar{y}) \in X_{ad}$ and $J(\bar{u}, \bar{y}) \leq J(u, y)$ for all $(u, y) \in X_{ad}$. The definition of S yields the characterization of X_{ad}

$$(\tilde{u}, \tilde{y}) \in X_{ad} \quad \Longleftrightarrow \quad \tilde{u} \in U_{ad} \text{ and } \tilde{y} = S(\tilde{u}) \quad \text{for all } (\tilde{u}, \tilde{y}) \in V \times W.$$

In combination with the definition of J_{red} and the identity $S(\bar{u}) = \mathcal{S}(\bar{u})$, the characterization shows that the inequality above is equal to $J_{red}(\bar{u}) = J(\bar{u}, \mathcal{S}(\bar{u})) \leq J(u, \mathcal{S}(u)) = J_{red}(u)$ for all $u \in U_{ad}$. This condition is fulfilled if and only if $\bar{u}$ is a solution of (5.8). □

Proposition 5.2.6. *The reduced cost function J_{red} is twice continuously Fréchet differentiable at every $u \in V$. The first derivative $J'_{red}(u) \in \mathcal{L}(U, \mathbb{R})$ is given by*

$$J'_{red}(u)v = (\mathcal{S}'(u)v, \mathcal{S}(u) - y_d)_{L^2(Q_T)^s} + \gamma(v, u - u_d)_U \quad \textit{for all } v \in U.$$

The second derivative $J''_{red}(u) \in \mathcal{L}(U, \mathcal{L}(U, \mathbb{R}))$ is defined by

$$J''_{red}(u)vw = (\mathcal{S}''(u)vw, \mathcal{S}(u) - y_d)_{L^2(Q_T)^s} + (\mathcal{S}'(u)v, \mathcal{S}'(u)w)_{L^2(Q_T)^s} + \gamma(v, w)_U \textit{ for all } v, w \in U.$$

Proof. First of all, we ensure that the components of J_{red} are twice continuously Fréchet differentiable. The observation operator $\mathcal{S}$ is the composition of the parameter-to-state map S and the linear and bounded operator E^s_W. Thus, Theorem 5.2.3 and the chain rule yield its twice continuous differentiability. Furthermore, the first derivative at $u \in V$ is equal to $\mathcal{S}'(u) = E^s_W \circ S'(u)$. An analogous result holds for $\mathcal{S}''(u)$. In particular, since E^s_W equals the identity map, the values of $\mathcal{S}'(u)$ and $\mathcal{S}''(u)$ are represented by the initial value problems specified in Theorem 5.2.3.

Moreover, an easy computation shows that the squared norm $\|\,.\,\|^2_H$ of a Hilbert space H is twice continuously Fréchet differentiable at every $h \in H$ with $\|\,.\,\|^{2\,\prime}_H(h)v = 2(v, h)_H$ and $\|\,.\,\|^{2\,\prime\prime}_H(h)vw = 2(v, w)_H$ for all $v, w \in H$.

Since the reduced cost function $J_{red} : V \to \mathbb{R}$ is equal to the composition

$$J_{red} = \frac{1}{2}\|(\,.\,) - y_d\|^2_{L^2(Q_T)^s} \circ \mathcal{S} + \frac{\gamma}{2}\|(\,.\,) - u_d\|^2_U,$$

it is twice continuously Fréchet differentiable according to the chain rule. Considering the derivative of the squared norm, we obtain that the first derivative $J'_{red}(u) \in \mathcal{L}(U, \mathbb{R})$ at $u \in V$ is given by

$$\begin{aligned} J'_{red}(u)v &= \left(\frac{1}{2}\|(\,.\,) - y_d\|^2_{L^2(Q_T)^s}\right)'(\mathcal{S}(u))[\mathcal{S}'(u)v] + \left[\left(\frac{\gamma}{2}\|(\,.\,) - u_d\|^2_U\right)'(u)\right]v \\ &= ((\,.\,), \mathcal{S}(u) - y_d)_{L^2(Q_T)^s}[\mathcal{S}'(u)v] + \gamma((\,.\,), u - u_d)_U[v] \end{aligned}$$

$$= (\mathcal{S}'(u)v, \mathcal{S}(u) - y_d)_{L^2(Q_T)^s} + \gamma(v, u - u_d)_U$$

for all $v \in U$. To compute the second derivative, we define the auxiliary functions

$$f_1 : V \to \mathcal{L}(U, L^2(Q_T)^s) \times L^2(Q_T)^s,\ f_1(u) := (\mathcal{S}'(u), \mathcal{S}(u) - y_d),$$
$$f_2 : \mathcal{L}(U, L^2(Q_T)^s) \times L^2(Q_T)^s \to \mathcal{L}(U, \mathbb{R}),\ f_2(\varphi, y) := (\varphi, y)_{L^2(Q_T)^s}.$$

Because of the differentiability of $\mathcal{S}$ and the product rule for the scalar product, the auxiliary functions are continuously Fréchet differentiable at $u \in V$ and $(\varphi, y) \in \mathcal{L}(U, L^2(Q_T)^s) \times L^2(Q_T)^s$, respectively, and the derivatives are given by

$$f_1'(u)v = (\mathcal{S}''(u)v, \mathcal{S}'(u)v) \quad \text{for all } v \in U,$$
$$f_2'(\varphi, y)(\psi, z) = (\varphi, z)_{L^2(Q_T)^s} + (\psi, y)_{L^2(Q_T)^s} \quad \text{for all } (\psi, z) \in \mathcal{L}(U, L^2(Q_T)^s) \times L^2(Q_T)^s.$$

Thus, the first summand of the first derivative, $J'_{red1} := f_2 \circ f_1 : V \to \mathcal{L}(U, \mathbb{R})$, is continuously Fréchet differentiable at $u \in V$ and

$$J''_{red1}(u)v = f_2'(f_1(u))f_1'(u)v = (\mathcal{S}'(u), \mathcal{S}'(u)v)_{L^2(Q_T)^s} + (\mathcal{S}''(u)v, \mathcal{S}(u) - y_d)_{L^2(Q_T)^s}$$

for all $v \in U$. The assertion about the second derivative of the second summand of J_{red} is a direct consequence of the result about squared Hilbert space norms indicated above. □

5.2.2 First and second order conditions for optimal parameters

On the basis of the equivalent formulation (5.8) of the parameter identification problem, we can formulate conditions for locally optimal parameters. A parameter $\bar{u} \in U_{ad}$ is called locally optimal for (5.1) and (u_d, y_d) if it is optimal in a neighborhood of $\bar{u}$, i.e., if a constant $\varepsilon > 0$ exists such that

$$J_{red}(\bar{u}) \le J_{red}(u) \quad \text{for all } u \in U_{ad} \text{ with } \|u - \bar{u}\|_U \le \varepsilon.$$

The admissible set U_{ad} is convex by assumption, and J_{red} is twice continuously Fréchet differentiable at every element of the superset V of U_{ad} due to Proposition 5.2.6. Thus, Theorem 4.23 of Tröltzsch [26] is applicable to the optimization problem (5.8). It states that $\bar{u} \in U_{ad}$ is locally optimal for (5.1) and (u_d, y_d) if the first order condition (variational inequality)

$$J'_{red}(\bar{u})(u - \bar{u}) \ge 0 \quad \text{for all } u \in U_{ad} \tag{5.9}$$

and the second order condition

$$J''_{red}(\bar{u})u^2 \ge \delta \|u\|_U^2 \quad \text{for all } u \in U \tag{5.10}$$

with a constant $\delta > 0$ are fulfilled. According to Tröltzsch [26, Lemma 2.21], the variational inequality (5.9) is a necessary condition for (globally) optimal parameters. This is already true for a Gâteaux differentiable cost function J_{red}.

In the remainder of this section, we regard the optimality conditions (5.9) and (5.10) more closely. Concerning (5.10), Proposition 5.2.6 yields

Result 5.2.7 (Second order condition)**.** *The second order condition* (5.10) *for a parameter* $\bar{u} \in U_{ad}$ *has the form*

$$(\mathcal{S}''(\bar{u})u^2, \mathcal{S}(\bar{u}) - y_d)_{L^2(Q_T)^s} + \|\mathcal{S}'(\bar{u})u\|^2_{L^2(Q_T)^s} + \gamma\|u\|^2_U \geq \delta\|u\|^2_U \quad \textit{for all } u \in U$$

with a constant $\delta > 0$.

The first order condition

In addition to inserting the definition of J_{red}, we reformulate the variational inequality (5.9) using the solution of an initial value problem ("state") and the solution of a terminal value problem ("adjoint state"). The set containing the variational inequality and the two problems is called optimality system. The representation in the form of an optimality system has the advantage that all information needed to compute the variational inequality is included.

To determine the optimality system, let $\bar{u} \in U_{ad}$. According to Proposition 5.2.6, the variational inequality (5.9) is equal to

$$(\mathcal{S}'(\bar{u})(u - \bar{u}), \mathcal{S}(\bar{u}) - y_d)_{L^2(Q_T)^s} + \gamma(u - \bar{u}, \bar{u} - u_d)_U \geq 0 \quad \text{for all } u \in U_{ad}.$$

To combine both summands, we express the $L^2(Q_T)^s$-scalar product on the left-hand side by means of the scalar product in the parameter space U. To this end, we use the "adjoint state" $p \in W(0,T)^s$. The following considerations prepare the definition of the adjoint state as the solution of a terminal value problem called adjoint equation. The actual definition is given in Theorem 5.2.9.

Hypothesis 5.2.1 claims that the domain of definition of the reaction term's partial derivative with respect to y can be extended to $L^2(0,T;H^1(\Omega))^s$. Being more precise, it is assumed that the operator

$$\hat{F} : L^2(0,T;H^1(\Omega))^s \to L^2(0,T;H^1(\Omega)^*)^s \text{ with } \hat{F}|_Y = F'_y(\bar{u}, S(\bar{u}))$$

exists and that the elements $\hat{F}(t)$ of the generating family satisfy a Lipschitz condition for almost every t.

We proceed with the definition of the adjoint equation's summands. For almost every t, the generating operators $B^s(t)$ and $\hat{F}(t) : H^1(\Omega)^s \to (H^1(\Omega)^*)^s$ are linear and bounded according to Lemma 1.4.2 and Hypothesis 5.2.1, respectively. Therefore, the adjoint operators $B^*(t)$ and $F^*(t)$ exist (cf. Rudin [22, Theorem 4.10]). Since the space $H^1(\Omega)^s$ is reflexive, the adjoints' domain of definition $(H^1(\Omega)^{**})^s$ can be identified with $H^1(\Omega)^s$. Consequently, the adjoints are defined by

$$\begin{aligned}
B^*(t) &: H^1(\Omega)^s \to (H^1(\Omega)^*)^s, \quad \langle B^*(t)(p), h\rangle_{(H^1(\Omega)^*)^s} := \langle B^s(t)(h), p\rangle_{(H^1(\Omega)^*)^s}, \\
F^*(t) &: H^1(\Omega)^s \to (H^1(\Omega)^*)^s, \quad \langle F^*(t)(p), h\rangle_{(H^1(\Omega)^*)^s} := \langle \hat{F}(t)(h), p\rangle_{(H^1(\Omega)^*)^s}
\end{aligned}$$

for all $p, h \in H^1(\Omega)^s$. The families $(B^*(t))_t$ and $(F^*(t))_t$ generate operators B^* and F^* from $L^2(0,T;H^1(\Omega))^s$ to $L^2(0,T;H^1(\Omega)^*)^s$ which are well-defined according to Lemma 1.4.2 and Hypothesis 5.2.1, respectively.

The families' dependence on time, which has not been regarded so far, is represented by the operators $\bar{B}^* : [0,T] \to \mathcal{L}(H^1(\Omega)^s, (H^1(\Omega)^*)^s)$ with $\bar{B}^*(t) := B^*(t)$ and $\bar{F}^*$ defined in an analogous way. We show that both $\bar{B}^*$ and $\bar{F}^*$ belong to $L^2(0,T;\mathcal{L}(H^1(\Omega)^s, (H^1(\Omega)^*)^s))$. First, Lemma 1.4.2(1) gives

$$\|\bar{B}^*(t)\|_{\mathcal{L}(H^1(\Omega)^s,(H^1(\Omega)^*)^s)} \le C_B.$$

Second, the definitions of $\bar{F}^*$ and $F^*(t)$ as well as the Lipschitz condition for $\hat{F}(t)$ yield

$$\|\bar{F}^*(t)\|_{\mathcal{L}(H^1(\Omega)^s,(H^1(\Omega)^*)^s)} = \sup_{y,w} \frac{\langle F^*(t)(y), w\rangle_{(H^1(\Omega)^*)^s}}{\|y\|_{H^1(\Omega)^s}\|w\|_{H^1(\Omega)^s}} = \sup_{y,w} \frac{\langle \hat{F}(t)(w), y\rangle_{(H^1(\Omega)^*)^s}}{\|y\|_{H^1(\Omega)^s}\|w\|_{H^1(\Omega)^s}} \le L'.$$

The upper bounds are constants and therefore quadratically integrable with respect to time. The operators $\bar{B}^*$ and $\bar{F}^*$ will appear in the proof of Theorem 5.2.9 below.

The following corollary of the existence theorem 2.2.1 will be used to prove the existence of an adjoint state.

Corollary 5.2.8. *All statements of Theorem 2.2.1 and Proposition 2.2.2 remain valid if B^s is replaced by an operator that fulfills the conditions (1)-(3) and (5) of Lemma 1.4.2. The same is true if the assumption (2) of Theorem 2.2.1 holds and the Lipschitz condition for $F_1(t)$ is replaced by the following properties: Given an arbitrary $\varepsilon > 0$, there exists a positive constant C_1 in such a way that*

$$|\langle F_1(z_1(t)) - F_1(z_2(t)), z(t)\rangle| \le C_1\|z(t)\|^2_{\Omega^s} + \varepsilon\|z(t)\|^2_{H^1(\Omega)^s} \tag{5.11}$$

holds for all $z_1, z_2 \in Y$ with $z := z_1 - z_2$. Furthermore, $F_1(t) : \Lambda \to (H^1(\Omega)^*)^s$ is continuous almost everywhere and bounded independently of t.

Proof. The first statement follows from the fact that the proofs of both Theorem 2.2.1 and Proposition 2.2.2 use no other properties of B^s than (1)-(3) and (5) of Lemma 1.4.2.

To prove the second statement, we peruse both proofs and show that all conclusions involving the Lipschitz condition for $F_1(t)$ are still valid under the alternative assumptions.

In the proof of Proposition 2.2.2, the Lipschitz condition appears twice, contributing to Equation (2.5) on page 24 and to Equation (2.10) on page 26. Given the alternative assumptions, Equation (2.5) holds because it is equal to (5.11). Equation (2.10) is valid since

$F_1(t)$ is continuous and bounded independently of t.

We proceed with the proof of Theorem 2.2.1. In connection with the assumption (2), the Lipschitz condition appears only once on page 28. The continuity of $F_1(t)$ which is proved here is a part of the alternative assumptions. □

In the next theorem, we define the adjoint equation and prove that it is solvable.

Theorem 5.2.9. *The terminal value problem, called adjoint equation,*

$$\begin{aligned} -p' + B^*(p) + F^*(p) &= \mathcal{S}(\bar{u}) - y_d \\ p(T) &= 0 \end{aligned} \tag{5.12}$$

has a unique solution $p \in W(0,T)^s$, called adjoint state. Here, the right-hand side $\mathcal{S}(\bar{u}) - y_d \in L^2(Q_T)^s$ is identified with an element of $L^2(0,T;H^1(\Omega)^*)^s$ in the sense of Lemma 1.4.1.

Proof. Instead of the terminal value problem (5.12), we solve an equivalent initial value problem obtained by a transformation with respect to time. We adapt this standard technique, used, for example, by Tröltzsch [26, Lemma 3.17], to operator equations. To this end, we define the bijective and continuously differentiable involution

$$\Phi : [0,T] \to [0,T], \quad \Phi(t) = T - t.$$

Furthermore, we regard the families consisting of the members $\tilde{B}^*(\tau) := (\bar{B}^* \circ \Phi^{-1})(\tau)$ and $\tilde{F}^*(\tau) := (\bar{F}^* \circ \Phi^{-1})(\tau)$, respectively, for every $\tau \in [0,T]$. Since these families have the same members as $(B^*(t))_t$ and $(F^*(t))_t$, they generate operators $\tilde{B}^*$ and $\tilde{F}^*$ from $L^2(0,T;H^1(\Omega))^s$ to $L^2(0,T;H^1(\Omega)^*)^s$. Similarly, we define $\tilde{r} := (\mathcal{S}(\bar{u}) - y_d) \circ \Phi^{-1} \in L^2(0,T;H^1(\Omega)^*)^s$.

By means of Corollary 5.2.8, applied to $L^2(0,T;H^1(\Omega))^s$ instead of Y and to $\tilde{F}^*$ instead of F_1, we show that the initial value problem

$$\tilde{p}' + \tilde{B}^*(\tilde{p}) + \tilde{F}^*(\tilde{p}) = \tilde{r} \quad \text{and} \quad \tilde{p}(0) = 0$$

has a unique solution $\tilde{p} \in W(0,T)^s$. As to the assumptions of Corollary 5.2.8, we observe that the space $W(0,T)^s$ is continuously embedded in $L^2(0,T;H^1(\Omega))^s$. The right-hand side $\tilde{r}$ belongs to $L^2(0,T;H^1(\Omega)^*)^s$. Since the adjoint operator $\tilde{B}^*$ is equal to B^s with inverted arguments, the statements (1)-(3) and (5) of Lemma 1.4.2 hold for $\tilde{B}^*$ as well. The linear operator $\tilde{F}^*$ fulfills $\tilde{F}^*(0) = 0$.

The assumption (2) of Theorem 2.2.1 additionally requires the weak continuity of $\tilde{F}^*$. Let $(y_n)_n$ be a sequence that converges weakly to y in $L^2(0,T;H^1(\Omega))^s$. Using the definitions of $\tilde{F}^*(\tau)$ and $\bar{F}^*$ as well as integration by substitution, we obtain for all $w \in L^2(0,T;H^1(\Omega))^s$

$$\begin{aligned} \langle \tilde{F}^*(y_n) - \tilde{F}^*(y), w \rangle_{L^2(0,T;H^1(\Omega)^*)^s} &= \int_0^T \langle \bar{F}^*(\Phi^{-1}(\tau))(y_n(\tau) - y(\tau)), w(\tau) \rangle_{(H^1(\Omega)^*)^s} d\tau \\ &= \int_0^T \langle \hat{F}(t)(w(\Phi(t))), y_n(\Phi(t)) - y(\Phi(t)) \rangle_{(H^1(\Omega)^*)^s} dt \end{aligned}$$

$$= \langle \hat{F}(w \circ \Phi), y_n \circ \Phi - y \circ \Phi \rangle_{L^2(0,T;H^1(\Omega)^*)^s}.$$

The last expression converges to zero since $\hat{F}(w \circ \Phi) \in L^2(0,T;H^1(\Omega)^*)^s$ and $y_n \circ \Phi \rightharpoonup y \circ \Phi$ in $L^2(0,T;H^1(\Omega))^s$ because of integration by substitution. This proves $\tilde{F}^*(y_n) \rightharpoonup \tilde{F}^*(y)$ in $L^2(0,T;H^1(\Omega)^*)^s$ since $L^2(0,T;H^1(\Omega))^s$ is reflexive. Thus, $\tilde{F}^*$ is weakly continuous.

We proceed with the remaining assumptions of Corollary 5.2.8. First, we estimate using the definition of $\tilde{F}^*(\tau)$ and the Lipschitz condition for $\hat{F}(t)$

$$\|\tilde{F}^*(\tau)(w)\|_{(H^1(\Omega)^*)^s} = \sup_{a \in H^1(\Omega)^s} \frac{\langle \hat{F}(\Phi^{-1}(\tau))(a), w\rangle_{(H^1(\Omega)^*)^s}}{\|a\|_{H^1(\Omega)^s}} \leq L'\|w\|_{H^1(\Omega)^s}$$

for all $w \in H^1(\Omega)^s$. This shows that $\tilde{F}^*(\tau)$ is bounded independently of τ. Being linear, $\tilde{F}^*(\tau)$ is also continuous for almost every τ.

To verify (5.11), let $\varepsilon > 0$ and $z_1, z_2 \in L^2(0,T;H^1(\Omega))^s$. We abbreviate $z := z_1 - z_2$. Using the linearity of $\tilde{F}^*(\tau)$ as well as Cauchy's inequality with ε in the final step, we obtain

$$\begin{aligned}
|\langle \tilde{F}^*(\tau)(z_1(\tau)) - \tilde{F}^*(\tau)(z_2(\tau)), z(\tau)\rangle_{(H^1(\Omega)^*)^s}| &= |\langle \hat{F}(\Phi^{-1}(\tau))(z(\tau)), z(\tau)\rangle_{(H^1(\Omega)^*)^s}| \\
&\leq L'\|z(\tau)\|_{\Omega^s}\|z(\tau)\|_{H^1(\Omega)^s} \leq \frac{L'^2}{4\varepsilon}\|z(\tau)\|^2_{\Omega^s} + \varepsilon\|z(\tau)\|^2_{H^1(\Omega)^s}.
\end{aligned}$$

The constant $C_1 := L'^2/(4\varepsilon)$ is positive.

Thus, Corollary 5.2.8, applied to $F_1 = \tilde{F}^*$ and $F_2 = 0$, yields a unique solution $\tilde{p} \in W(0,T)^s$ of the auxiliary initial value problem.

We demonstrate that $p := \tilde{p} \circ \Phi \in W(0,T)^s$ solves the reverse problem (5.12). The definition immediately yields $p(T) = \tilde{p}(\Phi(T)) = \tilde{p}(0) = 0$. Moreover, the chain rule implies

$$\tilde{p}'(\tau) = (p \circ \Phi^{-1})'(\tau) = \Phi^{-1\prime}(\tau)p'(\Phi^{-1}(\tau)) = -p'(\Phi^{-1}(\tau)).$$

Given $w \in L^2(0,T;H^1(\Omega))^s$, the composition $\tilde{w} := w \circ \Phi^{-1}$ belongs to $L^2(0,T;H^1(\Omega))^s$ as well. Since $\tilde{p}$ solves the forward equation, we obtain

$$\begin{aligned}
0 &= \int_0^T \langle \tilde{p}'(\tau) + \tilde{B}^*(\tilde{p})(\tau) + \tilde{F}^*(\tilde{p})(\tau) - \tilde{r}(\tau), \tilde{w}(\tau)\rangle_{(H^1(\Omega)^*)^s} d\tau \\
&= \int_0^T \langle -p'(\Phi^{-1}(\tau)) + \bar{B}^*(\Phi^{-1}(\tau))(p(\Phi^{-1}(\tau))) + \bar{F}^*(\Phi^{-1}(\tau))(p(\Phi^{-1}(\tau))) \\
&\qquad\qquad - (\mathcal{S}(\bar{u}) - y_d)(\Phi^{-1}(\tau)), w(\Phi^{-1}(\tau))\rangle_{(H^1(\Omega)^*)^s} d\tau \\
&= \int_0^T \langle -p'(t) + \bar{B}^*(t)(p(t)) + \bar{F}^*(t)(p(t)) - (\mathcal{S}(\bar{u}) - y_d)(t), w(t)\rangle_{(H^1(\Omega)^*)^s} dt.
\end{aligned}$$

In the second line, we insert the result about $\tilde{p}'(\tau)$ and the definitions of $\tilde{B}^*$, $\tilde{F}^*$, $\tilde{r}$ and $\tilde{w}$. In the last line, we use integration by substitution. According to the definitions of $\bar{B}^*$ and $\bar{F}^*$, it is possible to omit the bars. Since w is arbitrary and the terminal value condition holds,

$p \in W(0,T)^s$ is a solution of (5.12).

In addition, the last computation reveals that every solution p of the adjoint equation is associated with a solution $\tilde{p} := p \circ \Phi^{-1}$ of the auxiliary initial value problem. The uniqueness of $\tilde{p}$ and the bijectivity of Φ yield the uniqueness of the adjoint state. $\square$

Let $v \in U$ and $\bar{y} := S(\bar{u})$. We will use the adjoint state p to express $(\mathcal{S}'(\bar{u})v, \mathcal{S}(\bar{u}) - y_d)_{L^2(Q_T)^s}$ by means of the scalar product in U. According to Theorem 5.2.3 and the considerations at the beginning of the proof of Proposition 5.2.6, the derivative $h := \mathcal{S}'(\bar{u})v \in L^2(Q_T)^s$ actually belongs to $W(0,T)^s$ and solves

$$h' + B^s(h) + F_y'(\bar{u},\bar{y})h = [f'(\bar{u}) - F_u'(\bar{u},\bar{y})]v \quad \text{and} \quad h(0) = 0.$$

Both the adjoint state p and the derivative h are elements of $W(0,T)^s$. Inserting p as a test function into the equation for h and vice versa, we obtain

$$\int_0^T \{\langle h'(t), p(t)\rangle + \langle B^s(h), p(t)\rangle + \langle F_y'(\bar{u},\bar{y})h, p(t)\rangle\} dt = \langle [f'(\bar{u}) - F_u'(\bar{u},\bar{y})]v, p\rangle_{L^2(0,T;H^1(\Omega)^*)^s},$$

$$\int_0^T \{\langle -p'(t), h(t)\rangle + \langle B^*(p), h(t)\rangle + \langle F^*(p), h(t)\rangle\} dt = (\mathcal{S}(\bar{u}) - y_d, h)_{L^2(Q_T)^s}.$$

For the sake of clarity, we omit the dependence on time in some summands.

We prove that the left-hand sides of both equations are equal. This is clear for the second summands because of the definition of $B^*(t)$. Moreover, the definition of $F^*(t)$, the property of a generating family, and Hypothesis 5.2.1 yield

$$\langle F^*(t)(p(t)), h(t)\rangle = \langle \hat{F}(t)(h(t)), p(t)\rangle = \langle \hat{F}(h)(t), p(t)\rangle = \langle F_y'(\bar{u},\bar{y})h(t), p(t)\rangle$$

since $h \in W(0,T)^s$ belongs to Y. Finally, we apply integration by parts in $W(0,T)^s$ (cf. Theorem 1.1.2(3) with $V = H^1(\Omega)^s$) to the first summand of the first equation and insert the conditions $h(0) = 0$ and $p(T) = 0$. We obtain

$$\int_0^T \langle h'(t), p(t)\rangle dt = \int_0^T \langle -p'(t), h(t)\rangle dt + (h(T), p(T))_{\Omega^s} - (h(0), p(0))_{\Omega^s} = \int_0^T \langle -p'(t), h(t)\rangle dt.$$

The equality of the left-hand sides of both equations implies the equality of the right-hand sides, i.e.,

$$\langle [f'(\bar{u}) - F_u'(\bar{u},\bar{y})]v, p\rangle_{L^2(0,T;H^1(\Omega)^*)^s} = (\mathcal{S}(\bar{u}) - y_d, h)_{L^2(Q_T)^s}.$$

In combination with the definition of h, this equality yields

$$\begin{aligned}(\mathcal{S}'(\bar{u})v, \mathcal{S}(\bar{u}) - y_d)_{L^2(Q_T)^s} &= \langle [f'(\bar{u}) - F_u'(\bar{u},\bar{y})]v, p\rangle_{L^2(0,T;H^1(\Omega)^*)^s} \\ &= ([f'(\bar{u}) - F_u'(\bar{u},\bar{y})]^* p, v)_U.\end{aligned}$$

The last equality sign is due to the definition of $[f'(\bar{u}) - F'_u(\bar{u},\bar{y})]^* : L^2(0,T;H^1(\Omega))^s \to U$, the adjoint of the operator $[f'(\bar{u}) - F'_u(\bar{u},\bar{y})]$.

Using the last result, we transform the left-hand side of the variational inequality (5.9) into

$$\begin{aligned} J'_{red}(\bar{u})(u-\bar{u}) &= (\mathcal{S}'(\bar{u})(u-\bar{u}), \mathcal{S}(\bar{u}) - y_d)_{L^2(Q_T)^s} + \gamma(u-\bar{u}, \bar{u}-u_d)_U \\ &= ([f'(\bar{u}) - F'_u(\bar{u},\bar{y})]^* p, u-\bar{u})_U + \gamma(\bar{u}-u_d, u-\bar{u})_U \\ &= ([f'(\bar{u}) - F'_u(\bar{u},\bar{y})]^* p + \gamma(\bar{u}-u_d), u-\bar{u})_U \end{aligned}$$

for every $u \in U_{ad}$. Thus, the variational inequality is determined by the optimal parameter $\bar{u}$, the optimal state $\bar{y} = S(\bar{u})$, and the adjoint state p. The optimality system contains the variational inequality as well as the defining equations for $\bar{y}$ and p. To eliminate the parameter-to-state map from the formulation, we replace $\mathcal{S}(\bar{u})$ on the right-hand side of the adjoint equation by $\bar{y}$. This is possible because $\mathcal{S}(\bar{u})$ and $S(\bar{u})$ are equal.

Result 5.2.10 (Optimality system). *The first order necessary condition* (5.9) *for the parameter $\bar{u} \in U_{ad}$ corresponds to the variational inequality*

$$([f'(\bar{u}) - F'_u(\bar{u},\bar{y})]^* p + \gamma(\bar{u}-u_d), u-\bar{u})_U \geq 0 \quad \text{for all } u \in U_{ad}$$

with $\bar{y}, p \in W(0,T)^s$ solving the state equation and the adjoint equation

$$\begin{aligned} \bar{y}' + B^s(\bar{y}) + F(\bar{u},\bar{y}) &= f(\bar{u}) \qquad & -p' + B^*(p) + F^*(p) &= \bar{y} - y_d \\ \bar{y}(0) &= y_0 & p(T) &= 0. \end{aligned}$$

Special case: Constant parameters. Parameters in marine ecosystem models are often assumed to be constant. This implies that the parameter space is equal to $U = \mathbb{R}^{n_p}$. In this special case, $[f'(\bar{u}) - F'_u(\bar{u},\bar{y})]^* p$ can be identified with an element of $\mathbb{R}^{n_p}$. We will determine this element below.

Let $Z := L^2(0,T;H^1(\Omega)^*)^s$. First, the reaction term's derivative $F'_u(\bar{u},\bar{y}) \in \mathcal{L}(\mathbb{R}^{n_p}, Z)$ can be identified with the Jacobian matrix

$$F'_u(\bar{u},\bar{y}) = \begin{pmatrix} \partial_{u_1} F_1(\bar{u},\bar{y}) & \dots & \partial_{u_{n_p}} F_1(\bar{u},\bar{y}) \\ \vdots & \ddots & \vdots \\ \partial_{u_1} F_s(\bar{u},\bar{y}) & \dots & \partial_{u_{n_p}} F_s(\bar{u},\bar{y}) \end{pmatrix} \in L^2(0,T;H^1(\Omega)^*)^{s \times n_p}.$$

Let $v \in \mathbb{R}^{n_p}$. The definition of the adjoint operator yields

$$\big(F'_u(\bar{u},\bar{y})^* p, v\big)_{\mathbb{R}^{n_p}} = \langle F'_u(\bar{u},\bar{y}) v, p \rangle_Z = \sum_{j=1}^{s} \langle \sum_{i=1}^{n_p} \partial_{u_i} F_j(\bar{u},\bar{y}) v_i, p_j \rangle_{L^2(0,T;H^1(\Omega)^*)}$$

$$= \sum_{i=1}^{n_p} v_i \sum_{j=1}^{s} \langle \partial_{u_i} F_j(\bar{u}, \bar{y}), p_j \rangle_{L^2(0,T;H^1(\Omega)^*)} = \sum_{i=1}^{n_p} v_i \langle F'_{u_i}(\bar{u}, \bar{y}), p \rangle_Z.$$

Here, the expression $F'_{u_i}(\bar{u}, \bar{y}) \in Z$ describes the i-th column of the matrix $F'_u(\bar{u}, \bar{y})$ for all $i \in \{1, \dots, n_p\}$. The computation shows that $F'_u(\bar{u}, \bar{y})^* p \in \mathbb{R}^{n_p}$ can be identified with

$$F'_u(\bar{u}, \bar{y})^* p = \left(\langle F'_{u_1}(\bar{u}, \bar{y}), p \rangle_Z, \dots, \langle F'_{u_{n_p}}(\bar{u}, \bar{y}), p \rangle_Z \right).$$

Like $F'_u(\bar{u}, \bar{y})$, the derivative $f'(\bar{u})$ belongs to $\mathcal{L}(\mathbb{R}^{n_p}, Z)$. Thus, it is represented by an equivalent of the Jacobian matrix above with the entries $\partial_{u_i} f_j(\bar{u})$ instead of $\partial_{u_i} F_j(\bar{u}, \bar{y})$ for all $i \in \{1, \dots, n_p\}$ and $j \in \{1, \dots, s\}$. The same arguments as above show that $f'(\bar{u})^* p \in \mathbb{R}^{n_p}$ can be identified with

$$f'(\bar{u})^* p = \left(\langle f'_{u_1}(\bar{u}), p \rangle_Z, \dots, \langle f'_{u_{n_p}}(\bar{u}), p \rangle_Z \right).$$

The expression $f'_{u_i}(\bar{u})$ describes the i-th column of the matrix $f'(\bar{u})$ for all $i \in \{1, \dots, n_p\}$.

5.3 Optimality conditions in the periodic case

In this section, we investigate optimality conditions for the minimization problem (5.2) with a periodic initial value condition, i.e., $A(y) = y(T) - y(0)$. In this case, it is not realistic to assume unique solvability of the model equation because important model classes, such as models of *N-DOP* type, lack this property. Thus, we cannot directly transfer the proceeding of Section 5.2 based on Theorem 4.23 of Tröltzsch [26].

An alternative result about a first order necessary condition is given by Zowe and Kurcyusz [31]. However, in the case of models of *N-DOP* type, this approach fails as well because we are unable to prove the required regularity condition. This condition involves periodic solutions of a variant of the model equation with general, inhomogeneous right-hand sides. However, the available existence result Theorem 3.2.1 covers only right-hand sides fulfilling the conservation of mass condition.

To formulate optimality conditions nonetheless, we regard an alternative optimization problem with a transient instead of a periodic model equation. The newly introduced initial value becomes an additional parameter which is considered optimal if its difference to the terminal value of the model equation's solution is minimal. Thus, optimal parameters are associated with an approximately periodic solution of the model equation. The alternative optimization problem can be treated with the methods of Section 5.2.

5.3.1 Formulation of the alternative parameter identification problem

In this section, we use the terminology of Section 5.1 and postulate Hypothesis 5.1.1.

The alternative optimization problem includes the side condition $e(u, y) = 0$ and $y(0) =$

y_0. The initial value y_0 is regarded as an additional parameter in the Hilbert space $L^2(\Omega)^s$. The set of admissible initial values $I_{ad} \subseteq L^2(\Omega)^s$ is assumed to be convex and bounded. In case of models of *N-DOP* type, the boundedness is not a strong restriction as long as I_{ad} is chosen according to the upper bound given in Result 3.2.6 on page 46.

Considering the aim that an optimal initial value should be close to the terminal value of the model equation's solution, we define the alternative cost function $\tilde{J} : U \times L^2(\Omega)^s \times L^2(Q_T)^s \to \mathbb{R}$ by

$$\tilde{J}(u, y_0, y) := \frac{1}{2}\|y - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2}\|u - u_d\|^2_U + \frac{\varepsilon}{2}\|y(T) - y_0\|^2_{L^2(\Omega)^s}.$$

The coefficient $\varepsilon > 0$ controls the importance of the last summand in the optimization. With the definition $\tilde{X}_{ad} := \{(u, y_0, y) \in U_{ad} \times I_{ad} \times W(0,T)^s : e(u, y) = 0 \text{ and } y(0) = y_0\}$, we obtain the alternative optimization problem

$$\min_{(u,y_0,y)\in\tilde{X}_{ad}} \tilde{J}(u, y_0, y). \tag{5.13}$$

A pair $(\tilde{u}, \tilde{y}_0) \in U_{ad} \times I_{ad}$ is called optimal for (u_d, y_d) and a periodic state if there exists an element $\tilde{y} \in W(0,T)^s$ such that $(\tilde{u}, \tilde{y}_0, \tilde{y}) \in \tilde{X}_{ad}$ solves the optimization problem (5.13). The following theorem ensures that such optimal pairs exist.

Theorem 5.3.1. *Let the assumptions of either Theorem 5.1.4 or Corollary 5.1.5 be valid, modified in such a way that for every* $(u, y_0) \in U_{ad} \times I_{ad}$ *there exists* $y \in W(0,T)^s$ *such that* $(u, y_0, y) \in \tilde{X}_{ad}$*. Furthermore, the set of admissible states* $\tilde{Y}_{ad} := \{y \in W(0,T)^s : \exists (u, y_0) \in U_{ad} \times I_{ad} : (u, y_0, y) \in \tilde{X}_{ad}\}$ *is assumed to be bounded in* $W(0,T)^s$*. Hence, the minimization problem* (5.13) *has a solution.*

Proof. The space $\tilde{U} := U \times L^2(\Omega)^s$ is reflexive, and the set $\tilde{U}_{ad} := U_{ad} \times I_{ad}$ is bounded. Thus, we can transfer the proofs of Theorem 5.1.4 and Corollary 5.1.5 almost completely to the situation of problem (5.13) by simply replacing U by $\tilde{U}$ and U_{ad} by $\tilde{U}_{ad}$. Only the weak continuity of the initial value condition

$$A : L^2(\Omega)^s \times W(0,T)^s \to L^2(\Omega)^s, \quad A(y_0, y) = y(0) - y_0$$

requires a special consideration because A depends on the new parameter y_0. The proof of Theorem 5.1.4 yields the weak continuity of the first summand of A. The second summand is the identity map on $L^2(\Omega)^s$ which is obviously weakly continuous. □

5.3.2 Parameter-to-state map and reduced cost function

As in Section 5.2, we prepare the formulation of optimality conditions by defining a "reduced" version of problem (5.13) only depending on (u, y_0). To this end, we postulate Hypothesis 5.2.1 adapted to the optimization problem (5.13) in such a way that the model equation (5.1) has a unique, transient solution $y(u, y_0)$ for all initial values $y_0 \in L^2(\Omega)^s$ and all parameters $u \in V$. This assumption enables the definition of the parameter-to-state map

$$\tilde{S} : V \times L^2(\Omega)^s \to W(0,T)^s, \quad \tilde{S}(u, y_0) = y(u, y_0).$$

Theorem 5.3.2. *The parameter-to-state map $\tilde{S}$ is twice continuously Fréchet differentiable at every $\mathbf{u} = (u, y_0) \in V \times L^2(\Omega)^s$. The first derivative $\tilde{S}'(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, W(0,T)^s)$ maps $\mathbf{v} = (v, v_0) \in U \times L^2(\Omega)^s$ to the solution $h := \tilde{S}'(\mathbf{u})\mathbf{v}$ of*

$$\begin{aligned} h' + B^s(h) + F'_y(u,y)h &= f'(u)v - F'_u(u,y)v \\ h(0) &= v_0. \end{aligned}$$

The second derivative $\tilde{S}''(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, \mathcal{L}(U \times L^2(\Omega)^s, W(0,T)^s))$ maps $\mathbf{v} = (v, v_0), \mathbf{w} = (w, w_0) \in U \times L^2(\Omega)^s$ to the solution $a := \tilde{S}''(\mathbf{u})\mathbf{v}\mathbf{w}$ of

$$\begin{aligned} a' + B^s(a) + F'_y(u,y)a &= f''(u)vw - F''_{yu}(u,y)v\tilde{S}'(\mathbf{u})\mathbf{w} - F''_{yy}(u,y)\tilde{S}'(\mathbf{u})\mathbf{v}\tilde{S}'(\mathbf{u})\mathbf{w} \\ &\quad - F''_{uu}(u,y)vw - F''_{uy}(u,y)\tilde{S}'(\mathbf{u})\mathbf{v}w \\ a(0) &= 0. \end{aligned}$$

In both initial value problems, we use the abbreviation $y := \tilde{S}(\mathbf{u})$.

Proof. We proceed as in the proof of Theorem 5.2.3. First, we observe that the considerations concerning solvability at its beginning hold for inhomogeneous initial values as well. Thus, both initial value problems introduced in the theorem are uniquely solvable.

The auxiliary operator Φ is defined in the same way as in the proof of Theorem 5.2.3 with the exception that the domain of definition is extended to $(V \times L^2(\Omega)^s) \times W(0,T)^s$. Concerning the twice continuous Fréchet differentiability of Φ, we have to additionally regard the operator $(u, y_0, y) \mapsto -y_0$. Being linear and bounded, it is twice continuously Fréchet differentiable. The first derivative is the identity map on $L^2(\Omega)^s$ with a minus sign, and the second derivative is zero. Since the partial derivative with respect to y is independent of y_0, the extended domain of definition does not affect the result about its bijectivity obtained in the proof of Theorem 5.2.3. Thus, the implicit function theorem yields that $\tilde{S}$ is twice continuously Fréchet differentiable at every $(u, y_0) \in V \times L^2(\Omega)^s$.

To determine the first derivative of $\tilde{S}$, we compute the partial derivative of Φ at $\mathbf{u} = (u, y_0) \in V \times L^2(\Omega)^s$. Using the abbreviation $y := \tilde{S}(\mathbf{u})$, we obtain

$$\Phi'_{(u,y_0)}(\mathbf{u}, y)\mathbf{v} = (F'_u(u,y)v - f'(u)v, v_0) \in Z \times L^2(\Omega)^s \quad \text{for all } \mathbf{v} = (v, v_0) \in U \times L^2(\Omega)^s.$$

In combination with the definition of $\Phi'_y(\mathbf{u}, y)^{-1}$ according to (5.6), this identity proves the assertion about the first derivative. In addition, we observe that the first partial derivatives of Φ are independent of y_0. For this reason, the second partial derivatives are equal to the ones computed in the proof of Theorem 5.2.3 except for the notation ($\tilde{S}$ instead of S). This proves the assertion about the second derivative. $\square$

We proceed with the definition of a reduced version of the optimization problem (5.13). Since the solution y appears twice in the cost function $\tilde{J}$, two different observation operators are required to eliminate y.

Definition 5.3.3. *Let $\tilde{J}$ and $\tilde{S}$ be defined as above. We refer to the continuous embedding of $W(0,T)^s$ in $L^2(Q_T)^s$ as E_W^s and to the continuous embedding of $W(0,T)^s$ in $C([0,T];L^2(\Omega))^s$ as E_C^s (cf. Theorem 1.1.2(1)). Let the operator $E_T : C([0,T];L^2(\Omega))^s \to L^2(\Omega)^s$ be given as in the proof of Lemma 2.2.3.*

1. *We define the two observation operators*
   - $\tilde{\mathcal{S}} := E_W^s \circ \tilde{S} : V \times L^2(\Omega)^s \to L^2(Q_T)^s$,
   - $\tilde{g} := E_T \circ E_C^s \circ \tilde{S} : V \times L^2(\Omega)^s \to L^2(\Omega)^s$, $\tilde{g}(u,y_0) = [(E_C^s \circ \tilde{S})(u,y_0)](T)$.
2. *The function $\tilde{J}_{red} : V \times L^2(\Omega)^s \to \mathbb{R}$, defined by $\tilde{J}_{red} = \tilde{J} \circ (Id_U|_V, \tilde{g}, \tilde{\mathcal{S}})$, i.e.,*

$$\tilde{J}_{red}(u,y_0) = \frac{1}{2}\|\tilde{\mathcal{S}}(u,y_0) - y_d\|^2_{L^2(Q_T)^s} + \frac{\gamma}{2}\|u-u_d\|^2_U + \frac{\varepsilon}{2}\|\tilde{g}(u,y_0) - y_0\|^2_{L^2(\Omega)^s}$$

   for every $(u,y_0) \in V \times L^2(\Omega)^s$, is called reduced cost function.

The proof of Lemma 5.2.5, slightly adapted to the notation of this section, ensures that the minimization problem (5.13) is equivalent to the reduced problem

$$\min_{(u,y_0)\in U_{ad}\times I_{ad}} \tilde{J}_{red}(u,y_0). \tag{5.14}$$

The last preparatory result of this section concerns the Fréchet differentiability of $\tilde{J}_{red}$.

Proposition 5.3.4. *The reduced cost function $\tilde{J}_{red}$ is twice continuously Fréchet differentiable at every $\mathbf{u} = (u,y_0) \in V \times L^2(\Omega)^s$. The first derivative $\tilde{J}'_{red}(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, \mathbb{R})$ is given by*

$$\tilde{J}'_{red}(\mathbf{u})\mathbf{v} = (\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{v}, \tilde{\mathcal{S}}(\mathbf{u}) - y_d)_{L^2(Q_T)^s} + \gamma(v, u-u_d)_U + \varepsilon(\tilde{g}'(\mathbf{u})\mathbf{v} - v_0, \tilde{g}(\mathbf{u}) - y_0)_{L^2(\Omega)^s}$$

and the second derivative $\tilde{J}''_{red}(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, \mathcal{L}(U \times L^2(\Omega)^s, \mathbb{R}))$ by

$$\begin{aligned}\tilde{J}''_{red}(\mathbf{u})\mathbf{v}\mathbf{w} = {} & (\tilde{\mathcal{S}}''(\mathbf{u})\mathbf{v}\mathbf{w}, \tilde{\mathcal{S}}(\mathbf{u}) - y_d)_{L^2(Q_T)^s} + (\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{v}, \tilde{\mathcal{S}}'(\mathbf{u})\mathbf{w})_{L^2(Q_T)^s} + \gamma(v,w)_U \\ & + \varepsilon(\tilde{g}''(\mathbf{u})\mathbf{v}\mathbf{w}, \tilde{g}(\mathbf{u}) - y_0)_{L^2(\Omega)^s} + \varepsilon(\tilde{g}'(\mathbf{u})\mathbf{w} - w_0, \tilde{g}'(\mathbf{u})\mathbf{v})_{L^2(\Omega)^s}\end{aligned}$$

for all $\mathbf{v} = (v,v_0), \mathbf{w} = (w,w_0) \in U \times L^2(\Omega)^s$.

Proof. Both $\tilde{\mathcal{S}}$ and $\tilde{g}$ are compositions of the twice continuously Fréchet differentiable parameter-to-state map $\tilde{S}$ and operators which are linear and bounded. Thus, the observation operators are twice continuously Fréchet differentiable. The same holds for $\tilde{J}_{red} : V \times L^2(\Omega)^s \to \mathbb{R}$ because of the chain rule.

We determine the derivatives of $\tilde{J}_{red}$. The first two summands differ from J_{red} only in the domain of definition ($U \times L^2(\Omega)^s$ instead of U). Thus, the derivatives can be computed as in Proposition 5.2.6.

Let $\mathbf{u} = (u, y_0) \in V \times L^2(\Omega)^s$ and $\mathbf{v} = (v, v_0), \mathbf{w} = (w, w_0) \in U \times L^2(\Omega)^s$. The third summand of $\tilde{J}_{red}$ is given by the composition

$$\tilde{J}_{red3} := \frac{\varepsilon}{2} \| \, . \, \|^2_{L^2(\Omega)^s} \circ (\tilde{g} - Id_{L^2(\Omega)^s}) : V \times L^2(\Omega)^s \to \mathbb{R}.$$

To differentiate the functional $\tilde{J}_{red3}$, we modify the arguments concerning the first component of J_{red} in the proof of Proposition 5.2.6. According to the chain rule, the first derivative $\tilde{J}'_{red3}(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, \mathbb{R})$ is given by

$$\tilde{J}'_{red3}(\mathbf{u})\mathbf{v} = \left(\frac{\varepsilon}{2} \| \, . \, \|^2_{L^2(\Omega)^s} \right)' (\tilde{g}(\mathbf{u}) - y_0)[\tilde{g}'(\mathbf{u})\mathbf{v} - v_0] = \varepsilon(\tilde{g}'(\mathbf{u})\mathbf{v} - v_0, \tilde{g}(\mathbf{u}) - y_0)_{L^2(\Omega)^s}.$$

To compute the second derivative of $\tilde{J}_{red3}$, we define the auxiliary functions

$$f_1 : V \times L^2(\Omega)^s \to \mathcal{L}(U \times L^2(\Omega)^s, L^2(\Omega)^s) \times L^2(\Omega)^s, \; f_1(\mathbf{x}) := (\tilde{g}'(\mathbf{x}) - Id_{L^2(\Omega)^s}, \tilde{g}(\mathbf{x}) - y_0),$$
$$f_2 : \mathcal{L}(U \times L^2(\Omega)^s, L^2(\Omega)^s) \times L^2(\Omega)^s \to \mathcal{L}(U \times L^2(\Omega)^s, \mathbb{R}), \; f_2(\varphi, y) := \varepsilon(\varphi, y)_{L^2(\Omega)^s}.$$

The second auxiliary function is continuously Fréchet differentiable according to the product rule. The derivative of the first auxiliary function is $f_1'(\mathbf{u})\mathbf{v} = (\tilde{g}''(\mathbf{u})\mathbf{v}, \tilde{g}'(\mathbf{u})\mathbf{v})$. The chain rule yields that the first derivative $\tilde{J}'_{red3} = f_2 \circ f_1 : V \times L^2(\Omega)^s \to \mathcal{L}(U \times L^2(\Omega)^s, \mathbb{R})$ is continuously Fréchet differentiable with

$$\tilde{J}''_{red3}(\mathbf{u})\mathbf{v} = \varepsilon(\tilde{g}'(\mathbf{u}) - Id_{L^2(\Omega)^s}, \tilde{g}'(\mathbf{u})\mathbf{v})_{L^2(\Omega)^s} + \varepsilon(\tilde{g}''(\mathbf{u})\mathbf{v}, \tilde{g}(\mathbf{u}) - y_0)_{L^2(\Omega)^s}.$$

Thus, the assertions of the theorem are proved. □

Remark 5.3.5. *Let* $\mathbf{u} \in V \times L^2(\Omega)^s$. *The operators* E^s_W, E_T, *and* E^s_C *are linear and bounded. Thus,*

$$\tilde{\mathcal{S}}'(\mathbf{u}) = E^s_W \circ \tilde{S}'(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, L^2(Q_T)^s),$$
$$\tilde{g}'(\mathbf{u}) = E_T \circ E^s_C \circ \tilde{S}'(\mathbf{u}) \in \mathcal{L}(U \times L^2(\Omega)^s, L^2(\Omega)^s).$$

Let additionally $\mathbf{v} \in U \times L^2(\Omega)^s$. *The second line indicates that* $\tilde{g}'(\mathbf{u})\mathbf{v}$ *is the terminal value of* $\tilde{S}'(\mathbf{u})\mathbf{v}$. *Furthermore, the functions* $\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{v}$ *and* $\tilde{S}'(\mathbf{u})\mathbf{v}$ *are equal because* E^s_W *is the identity map. Comparable results hold for the second derivatives.*

5.3.3 Optimality conditions

Let $\mathbf{u} = (\tilde{u}, \tilde{y}_0) \in U_{ad} \times I_{ad}$. The pair $\mathbf{u}$ is called locally optimal for (u_d, y_d) and a periodic state if a constant $\varepsilon > 0$ exists such that

$$\tilde{J}_{red}(\mathbf{u}) \leq \tilde{J}_{red}(\mathbf{v}) \quad \text{for all } \mathbf{v} = (v, v_0) \in U_{ad} \times I_{ad} \text{ with } \|v - \tilde{u}\|_U^2 + \|v_0 - \tilde{y}_0\|_{L^2(\Omega)^s}^2 \leq \varepsilon^2.$$

Proposition 5.3.4 shows that $\tilde{J}_{red}$, defined on the superset $V \times L^2(\Omega)^s$ of the convex set $U_{ad} \times I_{ad}$, is twice continuously Fréchet differentiable. Thus, Theorem 4.23 of Tröltzsch [26] is applicable to the optimization problem (5.14). We obtain that the first and second order optimality conditions

$$\tilde{J}'_{red}(\mathbf{u})(\mathbf{v} - \mathbf{u}) \geq 0 \qquad \text{for all } \mathbf{v} \in U_{ad} \times I_{ad}, \tag{5.15}$$

$$\tilde{J}''_{red}(\mathbf{u})\mathbf{v}^2 \geq \delta \left(\|v\|_U^2 + \|v_0\|_{L^2(\Omega)^s}^2 \right) \qquad \text{for all } \mathbf{v} = (v, v_0) \in U \times L^2(\Omega)^s \tag{5.16}$$

with a constant $\delta > 0$ imply local optimality of $\mathbf{u}$.

Proposition 5.3.4 yields

Result 5.3.6 (Second order condition)**.** *The second order condition* (5.16) *is equal to*

$$(\tilde{\mathcal{S}}''(\mathbf{u})\mathbf{v}^2, \tilde{\mathcal{S}}(\mathbf{u}) - y_d)_{L^2(Q_T)^s} + \|\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{v}\|_{L^2(Q_T)^s}^2 + \gamma\|v\|_U^2 + \varepsilon(\tilde{g}''(\mathbf{u})\mathbf{v}^2, \tilde{g}(\mathbf{u}) - \tilde{y}_0)_{L^2(\Omega)^s}$$
$$+ \varepsilon(\tilde{g}'(\mathbf{u})\mathbf{v} - v_0, \tilde{g}'(\mathbf{u})\mathbf{v})_{L^2(\Omega)^s} \geq \delta \left(\|v\|_U^2 + \|v_0\|_{L^2(\Omega)^s}^2 \right)$$

for all $\mathbf{v} = (v, v_0) \in U \times L^2(\Omega)^s$ *with a constant* $\delta > 0$.

The first order condition

The aim of this section is the derivation of an optimality system containing the variational inequality (5.15). Let $\mathbf{w} := (w, w_0) \in U \times L^2(\Omega)^s$. As in Section 5.2.2, we express the derivative on the left-hand side of the variational inequality

$$\tilde{J}'_{red}(\mathbf{u})\mathbf{w} = (\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{w}, \tilde{\mathcal{S}}(\mathbf{u}) - y_d)_{L^2(Q_T)^s} + \gamma(w, \tilde{u} - u_d)_U + \varepsilon(\tilde{g}'(\mathbf{u})\mathbf{w} - w_0, \tilde{g}(\mathbf{u}) - \tilde{y}_0)_{L^2(\Omega)^s}$$

(cf. Proposition 5.3.4) by means of the scalar product in $U \times L^2(\Omega)^s$ and a suitable adjoint state. Let B^* and F^* be given as in Section 5.2.2 with $\hat{F}$ being the extension of $F'_y(\tilde{u}, \tilde{S}(\mathbf{u}))$ instead of $F'_y(\bar{u}, S(\bar{u}))$. We define the adjoint equation

$$\begin{aligned} -\tilde{p}' + B^*(\tilde{p}) + F^*(\tilde{p}) &= \tilde{\mathcal{S}}(\mathbf{u}) - y_d \\ \tilde{p}(T) &= \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0). \end{aligned} \tag{5.17}$$

Equation (5.17) differs from the transient adjoint equation (5.12) only in the inhomogeneous terminal value. The transient adjoint equation has a unique solution due to Theorem 5.2.9. However, this theorem, based on the general existence result in Theorem 2.2.1, holds for arbitrary terminal values in $L^2(\Omega)^s$. Thus, it yields also a unique solution $\tilde{p}$ of (5.17).

As in the transient case, we compare the equations for $h := \tilde{S}'(\mathbf{u})\mathbf{w}$ and $\tilde{p}$. For the sake of simplicity, we henceforth abbreviate the optimal state by $\tilde{y} := \tilde{S}(\mathbf{u})$. Inserting $\tilde{p}$ as a test function into the equation for h and vice versa, we obtain

$$\int_0^T \{\langle h'(t), \tilde{p}(t)\rangle + \langle B^s(h), \tilde{p}(t)\rangle + \langle F_y'(\tilde{u}, \tilde{y})h, \tilde{p}(t)\rangle\}dt = \langle [f'(\tilde{u}) - F_u'(\tilde{u}, \tilde{y})]w, \tilde{p}\rangle_{L^2(0,T;H^1(\Omega)^*)^s},$$
$$\int_0^T \{\langle -\tilde{p}'(t), h(t)\rangle + \langle B^*(\tilde{p}), h(t)\rangle + \langle F^*(\tilde{p}), h(t)\rangle\}dt = (\tilde{\mathcal{S}}(\mathbf{u}) - y_d, h)_{L^2(Q_T)^s},$$

leaving out the argument t in some summands. In addition, the initial and terminal value conditions $h(0) = w_0$ and $\tilde{p}(T) = \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0)$ hold.

As in Section 5.2.2, the second and the third summand of both equations coincide. The first summand of the first equation is transformed by means of integration by parts in $W(0,T)^s$ and the initial and terminal value conditions. Hence,

$$\begin{aligned}\int_0^T \langle h'(t), \tilde{p}(t)\rangle dt &= \int_0^T \langle -\tilde{p}'(t), h(t)\rangle dt + (h(T), \tilde{p}(T))_{\Omega^s} - (h(0), \tilde{p}(0))_{\Omega^s} \\ &= \int_0^T \langle -\tilde{p}'(t), h(t)\rangle dt + (h(T), \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0))_{\Omega^s} - (w_0, \tilde{p}(0))_{\Omega^s}.\end{aligned}$$

Therefore, the difference of the equations is equal to

$$\begin{aligned}&(h(T), \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0))_{\Omega^s} - (w_0, \tilde{p}(0))_{\Omega^s} \\ &\qquad = \langle [f'(\tilde{u}) - F_u'(\tilde{u}, \tilde{y})]w, \tilde{p}\rangle_{L^2(0,T;H^1(\Omega)^*)^s} - (\tilde{\mathcal{S}}(\mathbf{u}) - y_d, h)_{L^2(Q_T)^s}.\end{aligned}$$

According to Remark 5.3.5, $h(T)$ can be replaced by $\tilde{g}'(\mathbf{u})\mathbf{w}$ and h by $\tilde{\mathcal{S}}'(\mathbf{u})\mathbf{w}$. Additionally rearranging the summands, we conclude from the last identity

$$\begin{aligned}&(\tilde{\mathcal{S}}(\mathbf{u}) - y_d, \tilde{\mathcal{S}}'(\mathbf{u})\mathbf{w})_{L^2(Q_T)^s} + (\tilde{g}'(\mathbf{u})\mathbf{w}, \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0))_{\Omega^s} \\ &\qquad = \langle [f'(\tilde{u}) - F_u'(\tilde{u}, \tilde{y})]w, \tilde{p}\rangle_{L^2(0,T;H^1(\Omega)^*)^s} + (w_0, \tilde{p}(0))_{\Omega^s} \\ &\qquad = ([f'(\tilde{u}) - F_u'(\tilde{u}, \tilde{y})]^*\tilde{p}, w)_U + (\tilde{p}(0), w_0)_{\Omega^s}.\end{aligned}$$

The first line is equal to $\tilde{J}_{red}'(\mathbf{u})\mathbf{w} + (\varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0), w_0)_{\Omega^s} - \gamma(\tilde{u} - u_d, w)_U$. Thus, we arrive at the desired expression

$$\tilde{J}_{red}'(\mathbf{u})\mathbf{w} = ([f'(\tilde{u}) - F_u'(\tilde{u}, \tilde{y})]^*\tilde{p} + \gamma(\tilde{u} - u_d), w)_U + (\tilde{p}(0) - \varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0), w_0)_{L^2(\Omega)^s}.$$

We observe that $\varepsilon(\tilde{g}(\mathbf{u}) - \tilde{y}_0)$ could be replaced by $\tilde{p}(T)$.

As in Section 5.2.2, the results are summarized in an optimality system. Again, we replace the auxiliary operators $\tilde{\mathcal{S}}$ and $\tilde{g}$ using the optimal state $\tilde{y}$.

Result 5.3.7 (Optimality system)**.** *The necessary optimality condition* (5.15) *for the pair*

$(\tilde{u}, \tilde{y}_0) \in U_{ad} \times I_{ad}$ *corresponds to the variational inequality*

$$([f'(\tilde{u}) - F'_u(\tilde{u}, \tilde{y})]^* \tilde{p} + \gamma(\tilde{u} - u_d), v - \tilde{u})_U + (\tilde{p}(0) - \varepsilon(\tilde{y}(T) - \tilde{y}_0), v_0 - \tilde{y}_0)_{L^2(\Omega)^s} \geq 0$$

for all $(v, v_0) \in U_{ad} \times I_{ad}$ *with* $\tilde{y}, \tilde{p} \in W(0,T)^s$ *solving the state equation and the adjoint equation*

$$\begin{aligned} \tilde{y}' + B^s(\tilde{y}) + F(\tilde{u}, \tilde{y}) &= f(\tilde{u}) & \qquad -\tilde{p}' + B^*(\tilde{p}) + F^*(\tilde{p}) &= \tilde{y} - y_d \\ \tilde{y}(0) &= \tilde{y}_0 & \tilde{p}(T) &= \varepsilon(\tilde{y}(T) - \tilde{y}_0). \end{aligned}$$

5.4 Application to the PO_4-DOP model

In this section, we apply the results about parameter identification to the PO_4-DOP model (cf. Sections 4.2.2 and 4.2.3). The parameters in question are listed in Table 4.2.1 at the end of Section 4.2.2. First, we ensure that the basic assumptions of Hypotheses 1.2.1 and 5.1.1 are valid.

Concerning Hypothesis 1.2.1, we define the domain of definition $Y := L^3(Q_T)^2$ in which $W(0,T)^2$ is even compactly embedded (cf. Růžička [19, Corollary 3.98]). This space is convenient in connection with derivatives of superposition operators. The spaces Y and $\Lambda := L^3(\Omega)^2$ fulfill the property (1.1). The model contains $n_p := 7$ real parameters. Therefore, the parameter spaces are $U_i := \mathbb{R}$ for all $i \in \{1, \ldots, 7\}$ and $U = \mathbb{R}^7$. The last column of Table 4.2.1 suggests the definition $V := \mathbb{R}^6_{>0} \times (0,1) \subseteq U$. Sections 4.2.2 and 4.2.3 reveal that the restrictions of the PO_4-DOP model's reaction terms to $V \times Y$ fulfill the assumptions of Hypothesis 1.2.1.

Concerning Hypothesis 5.1.1, we define the admissible set U_{ad} by box constraints. Let $u_a, u_b \in \mathbb{R}^7$ with $0 < u_{a,i} \leq u_{b,i}$ for each $i \in \{1, \ldots, 7\}$ and $u_{b,7} < 1$. Then, the admissible set, defined by

$$U_{ad} := \{u \in \mathbb{R}^7 : u_{a,i} \leq u_i \leq u_{b,i} \quad \text{for all } i \in \{1, \ldots, 7\}\},$$

is a nonempty, closed, bounded, and convex subset of V. This kind of admissible set is used, for instance, by Prieß et al. [17, Section 5] for the identification of the PO_4-DOP model's seven parameters.

Furthermore, we consider the prescribed data $y_d \in L^2(Q_T)^2$ and the target parameter $u_d \in U_{ad}$. Let $\gamma \geq 0$ and $\varepsilon > 0$ be the controlling coefficients in the cost function. The initial value of a transient solution is denoted by $y_0 \in L^2(\Omega)^2$, and the initial value condition is abbreviated by $A(y) \in \{y(0) - y_0, y(0) - y(T)\}$ for all $y \in W(0,T)^2$.

5.4.1 Existence of optimal parameters

Let $y_0 \in L^2(\Omega)^2$ and $M \in \mathbb{R}$. We apply Corollary 5.1.5(3) to prove the existence of optimal parameters for the PO_4-DOP model and (u_d, y_d). The corollary is applicable because U is finite-dimensional and $W(0,T)^2$ is compactly embedded in $L^3(Q_T)^2$. In the following paragraphs, we verify the remaining assumptions of Theorem 5.1.4 and Corollary 5.1.5(3).

Reflexivity of U and solvability. The space U is a Hilbert space and therefore reflexive. Furthermore, Sections 4.4.1 and 4.4.2 ensure that the PO_4-DOP model has a transient solution with the initial value y_0 and a periodic solution with mass M for each fixed parameter vector $u \in U_{ad}$.

Boundedness of Y_{ad}. To show that the set of admissible states $Y_{ad} = \{y \in W(0,T)^2 : \exists u \in U_{ad} : e(u,y) = 0 \text{ and } A(y) = 0\}$ is bounded, we choose $y \in Y_{ad}$. The set is nonempty because of the solvability proved in the last paragraph. The solution y of the PO_4-DOP model is associated with a parameter $u = (\lambda, \alpha, K_P, K_I, K_W, \beta, \nu) \in U_{ad}$ and fulfills either the transient or the periodic initial value condition.

In the transient case, Proposition 2.2.2, applied to $F_2 = f = 0$, yields the estimate

$$\|y\|_{W(0,T)^2} \leq C\sqrt{1+\tilde{C}^2}\|y_0\|_{L^2(\Omega)^2}. \tag{5.18}$$

The initial value is independent of the parameters. The proof of Proposition 2.2.2 reveals that C and $\tilde{C}$ continuously depend on the Lipschitz constant L_1 and thus on the Lipschitz constants of d_1, d_2, and b_1, computed in Section 4.4.1. Therefore, we have to check that these constants, whose squares are equal to

$$2\left(\lambda^2 + \frac{2\alpha^2}{K_P^2}\left(1 + \left(\frac{h_{\max}}{\bar{h}_e} - 1\right)\beta^2(1-\nu)^2\right)\right), \quad 2\left(\lambda^2 + \frac{2\alpha^2\nu^2}{K_P^2}\right), \quad \text{and} \quad (1-\nu)^2\bar{h}_e\frac{2\alpha^2}{K_P^2},$$

are bounded independently of u. All Lipschitz constants are nonnegative. Furthermore, the parameters $\lambda, \beta, \nu, \alpha$ are each bounded from above by the associated component of u_b, the difference $1-\nu$ is strictly less than 1, and the parameter K_P is bounded from below by the positive lower bound u_{a3}. Thus, the box constraints provide upper bounds for the three Lipschitz constants.

In the periodic case, Result 3.2.6 states that the periodic solution y is bounded by a real number C_4. The computations preceding Result 3.2.6 reveal that C_4 continuously depends on the constant $\tilde{C}$ from Proposition 2.2.2 and the upper bound M_{rea} introduced in (3.1). All other components of C_4 are independent of the parameters. Thus, the proof is complete if $\tilde{C}$ and M_{rea} are bounded independently of the parameters. Concerning $\tilde{C}$, we checked this above. In Section 4.4.2, we showed that M_{rea} is the product of $M_{GEF} = \alpha \max\{\sqrt{|\Omega_1|}, \bar{h}_e(1-\nu)\sqrt{|\Omega'|}, (1-\nu)\beta\sqrt{|\Omega_2|}\}$ and a positive real number. The upper bound M_{GEF} is nonnegative and continuously depends on α, ν, and β. The parameters α and β are bounded from above by the corresponding components of u_b, and $1 - \nu$ is bounded by 1.

Demicontinuity. The right-hand sides of the PO_4-DOP model are zero and therefore demicontinuous. According to Section 4.4.1, the reaction terms are Lipschitz continuous for almost every t, and the Lipschitz constants are independent of t. Integrating the results of Section 4.4.1 with respect to t, we obtain the Lipschitz continuity and thus the continuity of $d : L^2(Q_T)^2 \to L^2(Q_T)^2$ and $b : L^2(Q_T)^2 \to L^2(\Sigma)^2$. The reaction terms remain continuous if the domain of definition is restricted to $L^3(Q_T)^2$ since this space is continuously embedded in $L^2(Q_T)^2$. Continuity implies demicontinuity.

5.4.2 Optimality conditions for the transient PO_4-DOP model

This section is dedicated to the question if the optimality conditions (5.9) and (5.10) hold in connection with locally optimal parameters of the transient PO_4-DOP model. Section 5.2 reveals that this is the case if U is a Hilbert space and Hypothesis 5.2.1 holds.

The finite-dimensional parameter space $U = \mathbb{R}^7$ is a Hilbert space. Moreover, Hypothesis 5.1.1 is valid (see above), and the PO_4-DOP model has a transient solution for each $u \in V = \mathbb{R}^6_{>0} \times (0, 1)$ (see Section 4.4.1).

The remaining claims of Hypothesis 5.2.1 include the twice continuous Fréchet differentiability of the reaction terms. According to Lemma 4.2.1, a saturation function is not twice continuously differentiable. For this reason, the uptake operator G, defined by means of the saturation function (4.2), cannot be twice continuously Fréchet differentiable either. We conclude that the assumptions of Hypothesis 5.2.1 are not fulfilled. However, it is possible to prove the continuous Fréchet differentiability of the reaction terms. In combination with the remaining assumptions of Hypothesis 5.2.1, this property ensures that an optimal parameter fulfills the first order condition (5.9) in the form of an optimality system.

In the first of the following two paragraphs, we prove the claims of Hypothesis 5.2.1 about the partial derivative with respect to y. The second one is dedicated to the continuous Fréchet differentiability. In both cases, we investigate the reaction terms $d : Y \to L^2(Q_T)^2$ and $b : Y \to L^2(\Sigma)^2$ instead of the corresponding operator F. According to Lemma 1.4.1, the operator is defined by a continuous embedding which does not affect differentiability.

Partial derivative with respect to y. In this paragraph, we investigate the reaction terms' partial derivative with respect to y concerning existence, continuity, and Lipschitz condition. We proceed gradually starting with the uptake operator $G : L^3(Q_T) \to L^2(Q_T)$ which is a superposition operator based on the real function in (4.2). Henceforth, we refer to the real function as $\mathcal{G}$ in order to express the difference between the function and the operator.

According to Appell and Zabrejko [1, Theorem 3.13], the superposition operator $G : L^3(Q_T) \to L^2(Q_T)$ is differentiable if $\mathcal{G}$ is differentiable with respect to y and if the derivative defines a superposition operator from $L^3(Q_T)$ to $L^6(Q_T)$.

Lemma 4.2.1 states that $\mathcal{G}$ is continuously differentiable with respect to y. The proof of this lemma reveals that the derivative is equal to

$$\mathcal{G}'_y : \mathbb{R} \times \Omega \times [0,T] \to \mathbb{R}, \quad \mathcal{G}'_y(y_1, x, t) = \frac{\alpha K_P}{(|y_1(x,t)| + K_P)^2} \frac{J(x,t)}{|J(x,t)| + K_I}.$$

We abbreviate insolation by $J(x,t) := I(x', t)\mathrm{e}^{-x_3 K_W}$ for all $(x,t) \in Q_T$. Since both fractions are bounded independently of (y_1, x, t), the real function $\mathcal{G}'_y$ defines a continuous superposition operator from $L^3(Q_T)$ to $L^6(Q_T)$. As a result, the operator $G : L^3(Q_T) \to L^2(Q_T)$ is Fréchet differentiable, and the derivative $G'(y_1) \in \mathcal{L}(L^3(Q_T), L^2(Q_T))$ at $y_1 \in L^3(Q_T)$ is given by

$$G'(y_1)v_1 := \frac{\alpha K_P}{(|y_1| + K_P)^2} \frac{J}{|J| + K_I} v_1 \quad \text{for all } v_1 \in L^3(Q_T).$$

The product of the fractions and v_1 still belongs to $L^2(Q_T)$ if $v_1 \in L^2(0,T; H^1(\Omega))$. In addition, the extension of $G'(y_1)$ to $L^2(0,T;H^1(\Omega))$ fulfills the desired Lipschitz condition. Both statements are due to the fractions' boundedness by the constant α/K_P which is independent of t. Furthermore, G' depends continuously on y_1.

The reaction terms' components E and $\bar{F}$ consist of an integral with respect to the third spatial variable over G, multiplied by an essentially bounded function with a suitable domain of definition. The following lemma is concerned with reaction terms of this type.

Lemma 5.4.1. *Let $\Psi \in \{Q_T, \Sigma\}$. Provided that $g \in L^\infty(\Psi)$, we define the nonlocal operator $F_g : L^3(Q_T) \to L^2(\Psi)$ at $y_1 \in L^3(Q_T)$ by*

$$F_g(y_1)(x,t) = g(x,t) \int_0^{h_e(x')} G(y_1)(x', \tilde{x}_3, t) d\tilde{x}_3 \quad \text{for almost all } (x,t) = (x', x_3, t) \in \Psi.$$

The operator F_g is continuously Fréchet differentiable at $y_1 \in L^3(Q_T)$, and the derivative, evaluated at $v_1 \in L^3(Q_T)$, is equal to

$$[F'_g(y_1)v_1](x,t) = g(x,t) \int_0^{h_e(x')} [G'(y_1)v_1](x', \tilde{x}_3, t) d\tilde{x}_3 \quad \text{for almost all } (x,t) = (x', x_3, t) \in \Psi.$$

The expression defining $F'_g(y_1)v_1$ still belongs to $L^2(\Psi)$ if $v_1 \in L^2(0,T;H^1(\Omega))$. The extension of $F'_g(y_1)$ to $L^2(0,T;H^1(\Omega))$ fulfills the desired Lipschitz condition.

Proof. The operator F_g is well-defined since the integrand is bounded independently of y_1, x', $\tilde{x}_3$, and t according to Lemma 4.2.1. Concerning differentiability, we consider the case $\Psi = \Sigma$ first and point out the difference to the case $\Psi = Q_T$ afterwards. Let $y_1, v_1 \in L^3(Q_T)$. Temporarily, we refer to the candidate for $F'_g(y_1)$ as A. Using the essential boundedness of g and h_e, Hölder's inequality, the definition of Ω_1, and $\Omega_1 \times [0,T] \subseteq Q_T$, we obtain

$$\|F_g(y_1 + v_1) - F_g(y_1) - Av_1\|_\Sigma^2 \le \|g\|^2 \int_0^T \int_{\Omega'} \left(\int_0^{h_e} [G(y_1 + v_1) - G(y_1) - G'(y_1)v_1] d\tilde{x}_3 \right)^2 dx' dt$$

$$\leq \|g\|^2 \int_0^T \int_{\Omega'} \bar{h}_e \int_0^{h_e} [G(y_1+v_1) - G(y_1) - G'(y_1)v_1]^2 d\tilde{x}_3 dx' dt$$
$$\leq \|g\|^2 \bar{h}_e \|G(y_1+v_1) - G(y_1) - G'(y_1)v_1\|^2_{L^2(Q_T)}.$$

Here, $\|g\|$ stands for the norm of g in $L^\infty(\Psi)$. In case $\Psi = Q_T$, we obtain the same estimate, multiplied by the additional coefficient $h_{\max}$. This is due to the fact that Q_T requires an additional integral over $[0, h(x')]$.

The last expression divided by $\|v_1\|_{L^3(Q_T)}$ converges to zero for $\|v_1\|_{L^3(Q_T)} \to 0$ since $G : L^3(Q_T) \to L^2(Q_T)$ is Fréchet differentiable. Thus, F_d is Fréchet differentiable as well. The Fréchet derivative A is continuous since G' depends continuously on y_1.

Since the fractions are bounded by a constant and g and h_e are essentially bounded, the expression

$$g \int_0^{h_e} \frac{\alpha K_P}{(|y_1(x_3)| + K_P)^2} \frac{J(x_3)}{|J(x_3)| + K_I} v_1(x_3) dx_3$$

belongs to $L^2(\Psi)$ for each $v_1 \in L^2(0,T;H^1(\Omega))$. The extension of $F_g'(y_1)$ to $L^2(0,T;H^1(\Omega))$ fulfills the required Lipschitz condition. To justify this, we realize that the extension has the same structure as $\bar{F}$ defined in Section 4.2.2. In Section 4.4.1, the Lipschitz condition for $\bar{F}$ is reduced to the Lipschitz continuity of G. In the same way, we deduce the Lipschitz condition for the extension of $F_g'(y_1)$ from the Lipschitz continuity of the extension of $G'(y_1)$. □

The reaction terms d and b of the PO_4-DOP model are composed of G, $\bar{F}$, and E as well as λId. The identity map Id from $L^3(Q_T)$ to $L^2(Q_T)$ is linear and bounded and thus continuously Fréchet differentiable. The derivative at $y_1 \in L^3(Q_T)$ is equal to the identity map. Its extension to $L^2(0,T;H^1(\Omega))$ is continuous and fulfills the Lipschitz condition.

The previous lemma implies that the operators $\bar{F} : L^3(Q_T) \to L^2(0,T;L^2(\Omega_2))$ and $E : L^3(Q_T) \to L^2(0,T;L^2(\Omega'))$ are continuously Fréchet differentiable. Furthermore, the derivatives have a linear extension to $L^2(0,T;H^1(\Omega))$ and fulfill the required Lipschitz condition. We proved above that all these properties hold for G as well. Thus, the reaction terms fulfill the desired properties concerning the partial derivative with respect to y.

Fréchet differentiability. This paragraph is dedicated to the continuous Fréchet differentiability of both the right-hand sides and the reaction terms of the PO_4-DOP model.

The right-hand sides are equal to zero and thus continuously Fréchet differentiable. To obtain a comparable result for the reaction terms, let $(\tilde{u}, \tilde{y}) \in V \times Y$. According to Proposition 4.14c) of Zeidler [28], it suffices to prove that all partial derivatives at $(\tilde{u}, \tilde{y})$ are existent and continuous. The last paragraph shows that this is true for the partial derivative with respect to y. For this reason, the current paragraph is concerned with the continuous differentiability with respect to each of the seven parameters.

Let $i \in \{1, \ldots, 7\}$. Since the parameters are real, the partial Fréchet derivative of d at $\tilde{u}_i$ can be identified with an element of $L^2(Q_T)^2$. To determine this element, we consider the real function $d_{i,x,t} : u_i \mapsto d(\tilde{u}_1, \ldots, u_i, \ldots, \tilde{u}_7, \tilde{y})(x,t)$ for a fixed $(x,t) \in Q_T$. If $d_{i,x,t}$ is continuously differentiable at $\tilde{u}_i$, the derivative enables the definition $\tilde{D} : (x,t) \mapsto d'_{i,x,t}(\tilde{u}_i)$. This function equals the partial derivative of d at $\tilde{u}_i$ if it belongs to $L^2(Q_T)^2$ and if the residual

$$\frac{1}{|h|}\|d(\tilde{u}_1, \ldots, \tilde{u}_i + h, \ldots, \tilde{u}_7, \tilde{y}) - d(\tilde{u}, \tilde{y}) - \tilde{D}h\|_{L^2(Q_T)^2}$$

converges to zero for $|h| \to 0$. An analogous consideration holds for b.

We prove the existence of $\tilde{D}$ and the convergence of the residual for $i = 1$ and $i = 3$. The other parameters can be treated similarly. In both cases, we consider only a relevant part δ of d instead of the whole reaction term.

First, we regard the remineralization rate $\tilde{u}_1 = \tilde{\lambda}$ and differentiate $\delta : \mathbb{R}_{>0} \to L^2(Q_T)$, $\lambda \mapsto \lambda\tilde{y}_2$. We immediately obtain the candidate $\tilde{D} = \tilde{y}_2 \in L^2(Q_T)$ for the Fréchet derivative. The expression $\|(\tilde{\lambda}+h)\tilde{y}_2 - \tilde{\lambda}\tilde{y}_2 - h\tilde{y}_2\|_{L^2(Q_T)}$ is equal to zero for every h. As a consequence, the residual converges to zero for $|h| \to 0$. The fact that the residual actually vanishes for every h is due to the linear dependence on λ. Therefore, similar considerations are valid for the derivatives with respect to $\tilde{u}_2 = \tilde{\alpha}$ and $\tilde{u}_7 = \tilde{\nu}$.

Second, we consider the half saturation rate $\tilde{u}_3 = \tilde{K}_P$ and differentiate $\delta : \mathbb{R}_{>0} \to L^2(Q_T)$, $K_P \mapsto (\tilde{\alpha}\tilde{y}_1)/(|\tilde{y}_1| + K_P)$. The quotient rule yields the candidate $\tilde{D} = -(\tilde{\alpha}\tilde{y}_1)/(|\tilde{y}_1| + \tilde{K}_P)^2$ which belongs to $L^2(Q_T)$. The continuous differentiability of $\delta_{3,x,t}$ at $\tilde{u}_3 = \tilde{K}_P$ implies that the residual in question converges almost everywhere in Q_T. We additionally show that it is dominated by a quadratically integrable function. Hence, Lebesgue's dominated convergence theorem yields the desired convergence in $L^2(Q_T)$. Abbreviating $\tilde{y}_1(x,t)$ by $\tilde{y}_1$, we calculate

$$\begin{aligned}
&\frac{1}{|h|}\left|\frac{\tilde{\alpha}\tilde{y}_1}{|\tilde{y}_1| + \tilde{K}_P + h} - \frac{\tilde{\alpha}\tilde{y}_1}{|\tilde{y}_1| + \tilde{K}_P} + \frac{\tilde{\alpha}\tilde{y}_1 h}{(|\tilde{y}_1| + \tilde{K}_P)^2}\right| \\
&\qquad = \frac{|\tilde{\alpha}\tilde{y}_1|}{|h|}\frac{|(|\tilde{y}_1| + \tilde{K}_P)^2 - (|\tilde{y}_1| + \tilde{K}_P)(|\tilde{y}_1| + \tilde{K}_P + h) + h(|\tilde{y}_1| + \tilde{K}_P + h)|}{(|\tilde{y}_1| + \tilde{K}_P)^2(|\tilde{y}_1| + \tilde{K}_P + h)} \\
&\qquad = \frac{|\tilde{\alpha}\tilde{y}_1|}{|h|}\frac{|-(|\tilde{y}_1| + \tilde{K}_P)h + h(|\tilde{y}_1| + \tilde{K}_P + h)|}{(|\tilde{y}_1| + \tilde{K}_P)^2(|\tilde{y}_1| + \tilde{K}_P + h)} = \frac{|\tilde{\alpha}\tilde{y}_1 h|}{(|\tilde{y}_1| + \tilde{K}_P)^2(|\tilde{y}_1| + \tilde{K}_P + h)}.
\end{aligned}$$

Choosing $|h| \leq \tilde{K}_P/2$, we estimate

$$(|\tilde{y}_1| + \tilde{K}_P + h)(|\tilde{y}_1| + \tilde{K}_P)^2 \geq (|\tilde{y}_1| + \tilde{K}_P)^3 - |h|(|\tilde{y}_1| + \tilde{K}_P)^2 \geq \frac{1}{2}(|\tilde{y}_1| + \tilde{K}_P)^3 \geq \frac{1}{2}\tilde{K}_P^3.$$

Thus, the residual is dominated by $\alpha|\tilde{y}_1(x,t)|/\tilde{K}_P^2$ almost everywhere for all sufficiently small h. The upper bound belongs to $L^2(Q_T)$.

The differentiability with respect to the half saturation constant $\tilde{u}_4 = \tilde{K}_I$ is shown analogously. The remaining parameters $\tilde{u}_6 = \tilde{\beta}$ and $\tilde{u}_5 = \tilde{K}_W$ are treated with similar arguments.

5.4.3 Optimality conditions for the periodic *PO_4-DOP* model

This section is concerned with the periodic *PO_4-DOP* model. We prove that optimal parameters of the associated transient auxiliary problem, introduced in Section 5.3, fulfill the variational inequality (5.15) in the form of an optimality system. As in the last section, we cannot expect the validity of the second order condition because the PO_4-DOP model's reaction terms are not twice continuously Fréchet differentiable.

Most of the required assumptions have been established before. At the beginning of Section 5.4, we deal with Hypothesis 5.1.1 and define the Hilbert space $U = \mathbb{R}^7$ as well as the domain of definition $V = \mathbb{R}^6_{>0} \times (0,1)$. According to the last section, the PO_4-DOP model's reaction terms are continuously Fréchet differentiable, and all claims of the original version of Hypothesis 5.2.1 (except for twice continuous Fréchet differentiability) hold. In addition, Section 4.4.1 shows that the PO_4-DOP model is uniquely solvable for all parameters $u \in V$ and all initial values in $L^2(\Omega)^2$.

Finally, we deal with the assumptions of Theorem 5.3.1. In Section 5.4.1, we prove that the PO_4-DOP model fulfills the assumptions of Corollary 5.1.5(3). Additionally, the solvability of the model equation for every $(u, y_0) \in U_{ad} \times I_{ad}$ and the boundedness of the set $\tilde{Y}_{ad} := \{y \in W(0,T)^2 : \exists (u, y_0) \in U_{ad} \times I_{ad} : (u, y_0, y) \in \tilde{X}_{ad}\}$ in $W(0,T)^2$ are required. The first property is regarded above. As to the second property, Equation (5.18) shows that a transient solution y of the PO_4-DOP model with the initial value y_0 fulfills

$$\|y\|_{W(0,T)^2} \leq C\sqrt{1 + \tilde{C}^2}\|y_0\|_{L^2(\Omega)^2}.$$

If y belongs to $\tilde{Y}_{ad}$, the initial value y_0 stems from the bounded set I_{ad}. Furthermore, the expression $C\sqrt{1 + \tilde{C}^2}$ is bounded according to Section 5.4.1. Thus, we obtain the boundedness of $\tilde{Y}_{ad}$.

5.4.4 Unique identifiability of parameters in the PO_4-DOP model

Because of its relatively low complexity, the PO_4-DOP model is suitable for tests in the context of parameter identification (see, for instance, Prieß et al. [17]). A test involves the identification of an optimal parameter for the PO_4-DOP model and the data $(u_d, y_d) \in X_{ad}$. This choice of data guarantees that (u_d, y_d) itself is a solution of the minimization problem (5.2) because $J(u_d, y_d) = 0$. Thus, the parameter u_d is optimal for the PO_4-DOP model and (u_d, y_d). In the context of a test, a numerical method is assessed by its ability to identify the known optimal parameter u_d. However, the explanatory power of such a test depends on whether the optimal parameter u_d is unique.

In case $\gamma > 0$, the optimal parameter u_d is unique irrespective of the model equation. To justify this, let $(\tilde{u}_d, \tilde{y}_d)$ be a minimum of (5.2). Then, the cost function J vanishes at $(\tilde{u}_d, \tilde{y}_d)$ because it vanishes at (u_d, y_d) as well. Thus, the two summands of $J(\tilde{u}_d, \tilde{y}_d)$ are equal to zero. This yields $\tilde{y}_d = y_d$ and $\tilde{u}_d = u_d$.

In the predominant case $\gamma = 0$, however, the considerations of the last paragraph yield only $\tilde{y}_d = y_d$. A corresponding result for the parameters requires the additional information that the equality of two states implies the equality of the associated parameters. In the transient case, this property corresponds to the injectivity of the parameter-to-state map S.

Parameters that fulfill this property are introduced in the following definition.

Definition 5.4.2. *For all $i \in \{1, \dots, 7\}$, the parameter u_i is called uniquely identifiable if the equality of two admissible states implies the equality of the associated i-th parameters.*

Investigation of unique identifiability

Let both components of $y_0 \in L^2(\Omega)^2$ be nontrivial. We regard the elements $u_1 = (\lambda_1, \alpha_1, K_{P1}, K_{I1}, K_{W1}, \beta_1, \nu_1)$ and $u_2 = (\lambda_2, \alpha_2, K_{P2}, K_{I2}, K_{W2}, \beta_2, \nu_2)$ of U_{ad} and the associated transient solutions $y(u_1) = (y_1, y_2)$ and $y(u_2)$ of the PO_4-DOP model with the initial value y_0. To investigate unique identifiability, we assume $y := y(u_1) = y(u_2)$.

The choice of the initial value ensures that the components y_1 and y_2 of the solution y are nontrivial. Furthermore, we assume that Ω_2 is nonempty and that

$$\int_0^{h_e} G(u_1, y_1) dx_3 \neq 0 \quad \text{in a subset } M \subseteq \Omega_2' \times [0, T] \text{ with } |M| > 0. \tag{5.19}$$

These preconditions enable us to draw conclusions about all seven parameters of the PO_4-DOP model.

By assumption, the solution y fulfills the equations

$$\int_0^T \{\langle y_1'(t), v_1(t)\rangle_{H^1(\Omega)^*} + B(y_1, v_1; t) + (d_1(u_i, y, t), v_1(t))_\Omega + (b_1(u_i, y, t), v_1(t))_\Gamma\} dt = 0$$
$$\int_0^T \{\langle y_2'(t), v_2(t)\rangle_{H^1(\Omega)^*} + B(y_2, v_2; t) + (d_2(u_i, y, t), v_2(t))_\Omega\} dt = 0$$

for $i \in \{1, 2\}$ and $v = (v_1, v_2) \in L^2(0, T; H^1(\Omega))^2$. Subtracting the equations with $i = 2$ from the equations with $i = 1$, we obtain

$$\int_0^T \{(d_1(u_1, y, t) - d_1(u_2, y, t), v_1(t))_\Omega + (b_1(u_1, y, t) - b_1(u_2, y, t), v_1(t))_\Gamma\} dt = 0 \tag{5.20}$$
$$\int_0^T (d_2(u_1, y, t) - d_2(u_2, y, t), v_2(t))_\Omega dt = 0. \tag{5.21}$$

To draw conclusions about identifiability, we restrict the integrands in (5.20) and (5.21) to different subsets of Q_T and Σ. To this end, we test the equations with an arbitrary v that vanishes everywhere except for the desired subset. Then, we apply the fundamental lemma of calculus of variations (see, for instance, Emmrich [4, Lemma 3.1.5]) to eliminate the integrals. Finally, we insert the definition of the reaction terms on the subset in question.

First, we restrict Equation (5.21) to $\Omega_2 \times [0, T]$ and obtain $\lambda_1 y_2 = \lambda_2 y_2$ almost everywhere. Since y_2 is nontrivial, we conclude $\lambda_1 = \lambda_2$. Thus, λ is uniquely identifiable.

Since $\lambda_1 = \lambda_2$, the restriction of Equation (5.20) to $\Omega_1 \times [0, T]$ yields

$$G(u_1, y_1) = G(u_2, y_1) \quad \text{almost everywhere.} \tag{5.22}$$

Here, unlike before, the parameters are included in the argument of G.

Combining the restriction of (5.21) to $\Omega_1 \times [0,T]$ with Equation (5.22), we conclude

$$\begin{aligned} 0 = \nu_1 G(u_1, y_1) - \nu_2 G(u_2, y_1) &= (\nu_1 - \nu_2) G(u_1, y_1) + \nu_2 (G(u_1, y_1) - G(u_2, y_1)) \\ &= (\nu_1 - \nu_2) G(u_1, y_1). \end{aligned}$$

Since α_1 and y_1 are nontrivial, so is $G(u_1, y_1)$. Thus, $\nu_1 = \nu_2$, i.e., ν is uniquely identifiable.

In the next step, we deal with the parameter β. Because of $1 - \nu \neq 0$, the restriction of (5.20) to the aphotic boundary $\Gamma_2 \times [0,T]$ yields

$$\begin{aligned} 0 &= \int_0^{h_e(x')} G(u_1, y_1) dx_3 \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_1} - \int_0^{h_e(x')} G(u_2, y_1) dx_3 \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_2} \\ &= \int_0^{h_e(x')} G(u_1, y_1) dx_3 \left(\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_1} - \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_2}\right) \\ &\qquad + \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_2} \int_0^{h_e(x')} (G(u_1, y_1) - G(u_2, y_1)) dx_3 \end{aligned}$$

for almost all (x', t) belonging to the set M from Equation (5.19). The arguments of the integrand in the last summand belong to $\Omega_1 \times [0,T]$. Thus, the whole summand vanishes because of (5.22). Since the integral over $G(u_1, y_1)$ is assumed to be nontrivial on M, we conclude

$$\left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_1} - \left(\frac{h(x')}{\bar{h}_e}\right)^{-\beta_2} = 0.$$

The fraction $q := \bar{h}_e / h(x')$ is strictly less than 1 since $(x', t) \in M$ implies $x' \in \Omega_2'$. The properties of the natural logarithm $\ln : \mathbb{R}_{>0} \to \mathbb{R}$ yield

$$\beta_1 \ln(q) = \ln(q^{\beta_1}) = \ln(q^{\beta_2}) = \beta_2 \ln(q).$$

The fact $\ln(q) \neq 0$ implies $\beta_1 = \beta_2$.

Provided that a certain condition is fulfilled, the remaining four parameters are not uniquely identifiable. We derive this condition from Equation (5.22) which is equal to

$$\alpha_1 \frac{y_1(x,t)}{|y_1(x,t)| + K_{P1}} \frac{I(x',t) \mathrm{e}^{-x_3 K_{W1}}}{I(x',t) \mathrm{e}^{-x_3 K_{W1}} + K_{I1}} = \alpha_2 \frac{y_1(x,t)}{|y_1(x,t)| + K_{P2}} \frac{I(x',t) \mathrm{e}^{-x_3 K_{W2}}}{I(x',t) \mathrm{e}^{-x_3 K_{W2}} + K_{I2}}$$

for almost all $(x,t) \in \Omega_1 \times [0,T]$. This equation provides information about the parameters only if $y_1(x,t) \neq 0$ and $I(x',t) > 0$. Therefore, we define the set $M_{y_1,I} \subseteq \Omega_1 \times [0,T]$ consisting of all pairs (x,t) with these properties. The assumptions ensure that $|M_{y_1,I}| > 0$.

Let $(x,t) \in M_{y_1,I}$ such that (5.22) holds. Omitting the arguments of y_1 and I, we conclude

$$\frac{\alpha_1}{\alpha_2} = \frac{|y_1| + K_{P1}}{y_1} \frac{I \mathrm{e}^{-x_3 K_{W1}} + K_{I1}}{I \mathrm{e}^{-x_3 K_{W1}}} \frac{y_1}{|y_1| + K_{P2}} \frac{I \mathrm{e}^{-x_3 K_{W2}}}{I \mathrm{e}^{-x_3 K_{W2}} + K_{I2}}$$

$$= \frac{|y_1| + K_{P1}}{|y_1| + K_{P2}} \frac{I\mathrm{e}^{-x_3 K_{W1}} + K_{I1}}{I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}} \mathrm{e}^{-x_3(K_{W2}-K_{W1})}$$

which is equivalent to

$$\frac{\alpha_1}{\alpha_2}(|y_1| + K_{P2})(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) = (|y_1| + K_{P1})(I\mathrm{e}^{-x_3 K_{W1}} + K_{I1})\mathrm{e}^{-x_3(K_{W2}-K_{W1})}.$$

Using the abbreviation $C := \alpha_1/\alpha_2$, we calculate

$$\begin{aligned}
0 &= C(|y_1| + K_{P2})(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) - (|y_1| + K_{P1})(I\mathrm{e}^{-x_3 K_{W1}} + K_{I1})\mathrm{e}^{-x_3(K_{W2}-K_{W1})} \\
&= C|y_1|(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) + CK_{P2}(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) \\
&\quad - |y_1|(I\mathrm{e}^{-x_3 K_{W2}} + K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})}) - K_{P1}(I\mathrm{e}^{-x_3 K_{W2}} + K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})}) \\
&= |y_1|\{C(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) - (I\mathrm{e}^{-x_3 K_{W2}} + K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})})\} \\
&\quad + CK_{P2}(I\mathrm{e}^{-x_3 K_{W2}} + K_{I2}) - K_{P1}(I\mathrm{e}^{-x_3 K_{W2}} + K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})}).
\end{aligned}$$

Rearranging the summands, we obtain

$$\begin{aligned}
&|y_1|\{((C-1)I - K_{I1}\mathrm{e}^{x_3 K_{W1}})\mathrm{e}^{-x_3 K_{W2}} + CK_{I2}\} \\
&\qquad = ((K_{P1} - CK_{P2})I + K_{P1}K_{I1}\mathrm{e}^{x_3 K_{W1}})\mathrm{e}^{-x_3 K_{W2}} - CK_{P2}K_{I2}.
\end{aligned} \tag{5.23}$$

In case $((C-1)I - K_{I1}\mathrm{e}^{x_3 K_{W1}})\mathrm{e}^{-x_3 K_{W2}} + CK_{I2} \neq 0$, we can divide Equation (5.23) by this expression. Expanding the resulting fraction by $\mathrm{e}^{x_3 K_{W2}}$, we obtain

$$|y_1| = \frac{(K_{P1} - CK_{P2})I + K_{P1}K_{I1}\mathrm{e}^{x_3 K_{W1}} - CK_{P2}K_{I2}\mathrm{e}^{x_3 K_{W2}}}{(C-1)I - K_{I1}\mathrm{e}^{x_3 K_{W1}} + CK_{I2}\mathrm{e}^{x_3 K_{W2}}}. \tag{5.24}$$

Equation (5.24) provides a condition for non-identifiability of the parameters α, K_P, K_I, and K_W.

Result 5.4.3. *At least one of the parameters α, K_P, K_I, and K_W is not uniquely identifiable if the following condition holds: There exists a parameter vector $u_1 \in U_{ad}$ such that the first component of the associated solution $y(u_1) = (y_1, y_2)$ fulfills*

$$|y_1(x,t)| = \frac{c_1 I(x',t) + c_2 e^{x_3 c_7} - c_3 e^{x_3 c_8}}{c_4 I(x',t) - c_5 e^{x_3 c_7} + c_6 e^{x_3 c_8}} \tag{5.25}$$

for almost all $(x,t) \in M_{y_1,I}$. Furthermore, it is possible to define admissible parameters α_2, K_{P2}, K_{I2}, and K_{W2} by means of the constants $c_1, \dots, c_8 \in \mathbb{R}$ such that (5.24) *holds.*

Proof. We assume that the condition holds. At least one of the parameters $\alpha_2, K_{P2}, K_{I2}, K_{W2}$ differs from the corresponding entry of u_1 since the denominator in (5.25) is nonzero. Thus, the parameter vector $u_2 := (\lambda_1, \alpha_2, K_{P2}, K_{I2}, K_{W2}, \beta_1, \nu_1) \in U_{ad}$ is different from u_1. The argumentation above shows that Equation (5.24) implies (5.22). In addition, the parameters λ_1, β_1 and ν_1 are equal in both vectors u_1 and u_2. Thus, we conclude $d(u_1, y(u_1)) =$

$d(u_2, y(u_1))$ and $b(u_1, y(u_1)) = b(u_2, y(u_1))$. This implies that u_1 and u_2 are both associated with the solution $y(u_1)$. □

Since we can neither prove nor disprove the condition given in Result 5.4.3, the four parameters α, K_P, K_I, and K_W may not be uniquely identifiable. This conclusion seems to support the results of Prieß et al. [17, Figure 5]. These authors are able to identify λ, β (here referred to as b) and ν (σ) satisfyingly. The computed optima for the remaining parameters differ from the desired values, some of them considerably. The most dissatisfying results are obtained for the half saturation constants K_P (K_N) and K_I.

Creating unique identifiability

Result 5.4.3 suggests that some parameters of the PO_4-DOP model may be unsuitable for the assessment of numerical methods because of their missing unique identifiability. In the following paragraphs, we present two possible ways to eliminate this deficit.

Identification of less parameters. Problematic parameters can be fixed with suitable values (obtained, for instance, by experiments or estimates). Thus, they become an invariable part of the reaction terms and leave both the vector u and the cost function. Accordingly, the optimization is reduced to the remaining, uniquely identifiable parameters.

Regarding the PO_4-DOP model, we suggest fixing the parameters associated with light, K_I and K_W. Then, the five parameters $\lambda, \alpha, K_P, \beta$ and ν remain to be identified via optimization in $U = \mathbb{R}^5$.

We justify our suggestion by proving the unique identifiability of the five variable parameters. To this end, let $u_i = (\lambda_i, \alpha_i, K_{Pi}, \beta_i, \nu_i)$ for $i \in \{1, 2\}$ be two admissible parameter vectors, each associated with the transient solution $y = (y_1, y_2)$. Again, we assume that y_1, y_2, and Ω_2 are nontrivial and that (5.19) holds. In the same way as above, we obtain $\lambda_1 = \lambda_2, \beta_1 = \beta_2$, and $\nu_1 = \nu_2$ as well as the equivalent of Equation (5.22)

$$\alpha_1 \frac{y_1(x,t)}{|y_1(x,t)| + K_{P1}} = \alpha_2 \frac{y_1(x,t)}{|y_1(x,t)| + K_{P2}} \quad \text{for almost every } (x,t) \in \Omega_1 \times [0,T] .$$

Restricted to the set $M_{y_1,I}$, this equation can be transformed into

$$\frac{\alpha_1}{\alpha_2} = \frac{|y_1(x,t)| + K_{P1}}{|y_1(x,t)| + K_{P2}} = 1 + \frac{K_{P1} - K_{P2}}{|y_1(x,t)| + K_{P2}}.$$

Since the left-hand side is constant, the same is true for the right-hand side. If the numerator on the right-hand side were nonzero, the fraction and thus the entire right-hand side would vary in $M_{y_1,I}$ because we excluded the only possible constant solution $y_1 = 0$. Thus, the numerator is equal to zero, i.e., $K_{P1} = K_{P2}$. As an immediate consequence, we obtain $\alpha_1 = \alpha_2$.

Introduction of new reaction terms. Suitable values for the non-identifiable parameters might be unavailable, or a fixation of single parameters might be undesirable for other reasons. In these cases, the reaction terms containing non-identifiable parameters can be replaced entirely. This procedure might yield new, artificial parameters which are not directly associated with the biogeochemical processes modeled.

The previous results indicate that non-identifiability, if existent, arises from the product of saturation functions. Therefore, we approximate the real saturation function $h : y_1 \mapsto \alpha y_1/(|y_1| + K_P)$, depending on the parameters α and K_P, by the function $g : y_1 \mapsto \mu \arctan(y_1)$ with one parameter μ. Figure 5.4.1 shows that the curves of both functions with appropriate parameter values behave similarly.

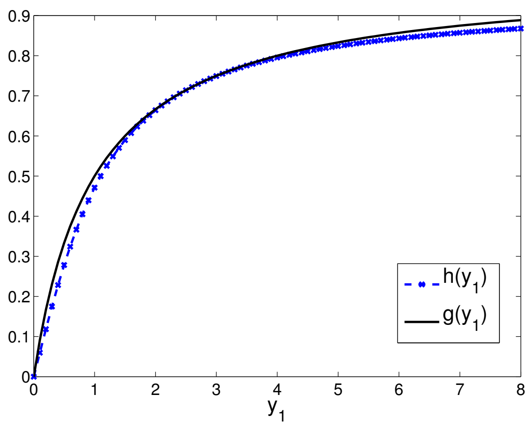

Figure 5.4.1: The saturation function h with $\alpha = K_P = 1$ compared to the function g with $\mu = 0.6$ on the interval $[0, 8]$.

Accordingly, the operator G in the PO_4-DOP model's reaction terms is replaced by

$$\tilde{G}(\mu, K_I, K_W, y_1) := \mu \arctan(y_1) \frac{I e^{-x_3 K_W}}{I e^{-x_3 K_W} + K_I}.$$

The altered model contains six parameters belonging to an appropriately adapted admissible set U_{ad}. In the remainder of this section, we prove that all of the six parameters are uniquely identifiable. To this end, let $u_i = (\lambda_i, \mu_i, K_{Ii}, K_{Wi}, \beta_i, \nu_i)$ for $i \in \{1, 2\}$ be admissible parameter vectors which are both associated with the transient solution $y = (y_1, y_2)$ of the altered model. As usual, we assume that y_1, y_2, and Ω_2 are nontrivial and that (5.19) holds. In the same way as above, we obtain $\lambda_1 = \lambda_2, \beta_1 = \beta_2$, and $\nu_1 = \nu_2$ as well as the equivalent of Equation (5.22)

$$\mu_1 \arctan(y_1(x,t)) \frac{I(x', t) e^{-x_3 K_{W1}}}{I(x', t) e^{-x_3 K_{W1}} + K_{I1}} = \mu_2 \arctan(y_1(x,t)) \frac{I(x', t) e^{-x_3 K_{W2}}}{I(x', t) e^{-x_3 K_{W2}} + K_{I2}}.$$

Restricted to the set $M_{y_1,I}$, this equation is equivalent to

$$\frac{\mu_1}{\mu_2} = \mathrm{e}^{-x_3(K_{W2}-K_{W1})} \frac{I(x',t)\mathrm{e}^{-x_3 K_{W1}} + K_{I1}}{I(x',t)\mathrm{e}^{-x_3 K_{W2}} + K_{I2}} = 1 + \frac{K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})} - K_{I2}}{I(x',t)\mathrm{e}^{-x_3 K_{W2}} + K_{I2}} \tag{5.26}$$

since $I(x',t) > 0$ and $\arctan(y_1(x,t)) \neq 0$ for all $(x,t) \in M_{y_1,I}$.

The right-hand side of (5.26) varies with x' if and only if the fraction is not equal to zero. Since the left-hand side is constant, the fraction vanishes, i.e., $K_{I1}\mathrm{e}^{-x_3(K_{W2}-K_{W1})} - K_{I2} = 0$. The right-hand side of the equivalent equation

$$\mathrm{e}^{-x_3(K_{W2}-K_{W1})} = \frac{K_{I2}}{K_{I1}}$$

is constant with respect to x_3. The same is true for the left-hand side if and only if $K_{W2} = K_{W1}$. This equality implies $K_{I2} = K_{I1}$. Finally, Equation (5.26) yields $\mu_1 = \mu_2$.

The function g, defined by means of the arc tangent, is one example for an approximation of the saturation function h. Alternatively, g could be defined by means of another, similarly shaped function ("sigmoid function"). Depending on the range of y_1, further alternatives might exist. For example, if the range is sufficiently small, a linear function provides an acceptable approximation of h.

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Erklärung

Hiermit versichere ich,

I. dass diese Arbeit – abgesehen von der Beratung durch den Betreuer Thomas Slawig – nach Inhalt und Form meine eigene ist,

II. dass Vorversionen einiger Teile dieser Arbeit bereits veröffentlicht wurden, nämlich

II.a. C. Roschat and T. Slawig: Mathematical analysis of a marine ecosystem model with nonlinear coupling terms and non-local boundary conditions, ArXiv e-prints, ArXiv:1403.4461, 2014.

II.b. C. Roschat and T. Slawig: Nontrivial Periodic Solutions of Marine Ecosystem Models of N-DOP type, ArXiv e-prints, ArXiv: 1409.7540, 2014.

II.c. C. Roschat and T. Slawig: Mathematical analysis of the PO4-DOP-Fe marine ecosystem model driven by 3-D ocean transport, ArXiv e-prints, ArXiv: 1501.05428, 2015.

III. dass kein Teil dieser Arbeit bereits einer anderen Stelle im Rahmen eines Prüfungsverfahrens vorgelegen hat,

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Christina Roschat
24. Februar 2016