Upscaling of processes involving rough boundaries

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Where innovation starts

1 Introduction

1.1 Upscaling

This thesis involves a type of problem that relates to upscaling, a process that typically involves two or more scales. In our case, we look at a domain with an oscillatory boundary with both amplitude and period ε. The size of the oscillations in this boundary (microscale) and the size of the domain (macroscale) provide us with these scales. Our goal will be to obtain effective equations only on the macroscale, where some information in these equations is carried over from the microscale. This process is called homogenization.
We will focus on the linear adsorption-desorption model. This model can be extended towards non-linear rates, or even discontinuous rates, as shown in [10], with applications in various fields. The ε-dependent problem P^{ε}, defined on a domain Ω^{ε} with oscillatory boundary Γ^{ε} will have a solution pair represented by $(u^{\varepsilon}, v^{\varepsilon})$. In this context, we assume u^{ε} to be a dissolved species in a fluid, defined in the domain, whereas v^{ε} will be the adsorbent defined only at the oscillatory boundary. Our upscaling problem will now be as follows:

Problem 1.1.1. *Derive a problem P in a simple domain Ω with a smooth and flat boundary Γ such that the solution (u, v) of problem P approximates the solution $(u^{\varepsilon}, v^{\varepsilon})$ of problem P^{ε}.*

It is clear that we will need to define Ω and Γ properly.
Imagine that we could solve Problem 1.1.1. The main question would be why we wanted this approximation in the first place. In general, the motivation for such an approximation is the following. In most cases we would like to solve the problem numerically because of the complexity of the problem and the fact that computers are in fact faster than humans when it comes to complex calculations. Here also lies the main issue of the original model - due to the oscillations in the boundary, the mesh size should be very small at these oscillations. From a practical point of view this makes the problem computationally very expensive.
The upscaling process of course solves this issue, however the simplification comes at a price. The simplification invokes corrections that we need to take into account.

Those corrections come in the form of modified boundary conditions. Also, the upscaling process should use some information from the original geometry. We will justify the upscaling process rigorously.

1.2 Thesis outline

The thesis is structured as follows. In Chapter 2 we will give relevant definitions, theorems, etc. that we will need in the remaining part of the thesis. In Chapter 3 we will discuss the adsorption and desorption model and provide the dimensionless form of that model. In Chapter 4 we will explain Rothe's method and apply it to the dimensionless model. In Chapter 5 we will discuss relevant unfolding techniques on our problem and in Section 5.4 we will apply them on our problem. Then we will discuss the numerical computations on our problem in Chapter 6. And in Chapter 7 we will state our conclusions and make recommendations with respect to possible future work.

2 Preliminaries

In this chapter, we introduce the theoretical concepts used in this thesis, such as Banach spaces, Hilbert spaces, Sobolev spaces and Bochner spaces. Furthermore, we will discuss some results in Hilbert and Banach spaces, that are commonly used throughout the following chapters. More on the given measures and integrals can be found in [16] (Chapters 4, 9 and 10), and for a more extensive introduction to the topic of weak derivatives and Sobolev Spaces we recommend the lecture notes [15].
In this chapter, the proofs of the stated theorems are omitted. For the proofs, we refer to [7] (Chapter 5, Appendices B and E), where one can also find a more detailed explanation of the measures and spaces discussed in this section.

2.1 Lebesgue measure

The Lebesgue measure describes a way of quantifying the size of certain subsets of $\Omega \subset \mathbb{R}^n$.

Definition 2.1.1. *A collection $\mathcal{M}$ of subsets of Ω is called a σ-algebra if*

- $\emptyset, \Omega \in \mathcal{M}$,
- $E \in \mathcal{M}$ *implies* $\Omega - E \in \mathcal{M}$,
- *if* $\{E_k\}_{k=1}^{\infty} \subset \mathcal{M}$, *then* $\bigcup_{k=1}^{\infty} E_k \in \mathcal{M}$ *and* $\bigcap_{k=1}^{\infty} E_k \in \mathcal{M}$.

On a σ-algeba one can define a measure based on the following:

Theorem 2.1.1. *There exist a σ-algebra $\mathcal{M}$ of subsets of Ω and a mapping $|.| : \mathcal{M} \to [0, \infty]$ with the following properties:*

- *Every open and therefore also every closed subset of Ω belong to $\mathcal{M}$.*
- *If B is a ball in Ω, then $|B|$ equals the n-dimensional volume of B.*

- *If* $\{E_k\}_{k=1}^{\infty} \subset \mathcal{M}$ *and* $\{E_k\}_{k=1}^{\infty}$ *are pairwise disjoint, then*

$$\left|\bigcup_{k=1}^{\infty} E_k\right| = \sum_{k=1}^{\infty} |E_k| .$$

- *If* $A \subseteq B$ *and* $B \in \mathcal{M}$ *and* $|B| = 0$*, then* $A \in \mathcal{M}$ *and* $|A| = 0$*.*

The sets in $\mathcal{M}$ *are called Lebesgue measurable sets and* $|\cdot|$ *is the* n*-dimensional Lebesgue measure.*

Definition 2.1.2. *A (positive) measure* μ *on a set* X *is a mapping* $\mu : \mathcal{M} \to [0, \infty]$ *defined on a* σ*-algebra* $\mathcal{M}$ *satisfying:*

- $\mu(\emptyset) = 0$
- *for any countable number of disjoint sets* $\left(A_j\right)_{j\in\mathbb{N}} \subset \mathcal{M}$*,*

$$\mu\left(\bigcup_{j\in\mathbb{N}} A_j\right) = \sum_{j\in\mathbb{N}} \mu\left(A_j\right)$$

If μ *is a measure on* X, $(X, \mathcal{M}, \mu)$ *is called a measure space.*

Definition 2.1.3. *Let* $(X, \mathcal{M}, \mu)$ *be a measure space. Let* $A_1, ..., A_n \in \mathcal{M}$ *be a sequence of measurable sets, and let* $a_1, ..., a_n$ *be a sequence of real numbers. A simple function* $f : \Omega \to \mathbb{R}$ *is of the form*

$$f(x) = \sum_{k=1}^{n} a_k \mathbf{1}_{A_k}(x)$$

where $\mathbf{1}_{A_k}$ *is the indicator function of the set* A_k*.*

Definition 2.1.4. *Let* $f : \Omega \to \mathbb{R}$*. We say* f *is a measurable function if* $f^{-1}(U) \in \mathcal{M}$ *for each open subset* $U \subset \mathbb{R}$*.*

This implies that if f is continuous, it is also measurable. Moreover the sum and product of two measurable functions are also measurable.

Guided by the idea that the Lebesgue integral should be the area between the graph of a function and the x-axis, we can define

$$\int \mathbf{1}_A d\mu = \mu(A)$$

for indicator functions and extend this definition to all positive simple functions by linearity.

Theorem 2.1.2. *Every measurable function $u : X \to \mathbb{R}$ is the pointwise limit of simple functions.*

This theorem tells us we can define the integral of any u in the space of positive measurable functions $\mathbb{M}^+$.

Definition 2.1.5. *We can observe that for all $u \in \mathbb{M}$, we can take $u = u^+ - u^-$ where both u^+ and $u^- \in \mathbb{M}$. In this case we call*

$$\int u d\mu := \int u^+ d\mu - \int u^- d\mu \in (-\infty, \infty)$$

the Lebesgue integral.

Definition 2.1.6. *A measurable function $f : \Omega \to \mathbb{R}$ where $(\Omega, (M), \mu)$ is a measure space is called summable if the Lebesgue integral of the absolute value of f exists and is finite. We can also say $f \in L^1(\Omega)$.*

2.2 Banach spaces and Hilbert spaces

Definition 2.2.1. *A Banach space is a vector space X over the field of real numbers $\mathbb{R}$ or complex numbers $\mathbb{C}$ which is equipped with a norm and which is complete with respect to that norm.*

Definition 2.2.2. *Suppose Ω is an open subset of $\mathbb{R}^n$ and $1 \leq p \leq \infty$. Suppose $f : \Omega \to \mathbb{R}$ is measurable, we define $L^p(\Omega)$ to be the linear space of all measurable functions $f : \Omega \to \mathbb{R}$ for which $||f||_{L^p(\Omega)} < \infty$. where the $L^p(\Omega)$ norm is defined as:*

$$||f||_{L^p(\Omega)} := \begin{cases} \left(\int\limits_\Omega |f|^p \, dx \right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty \\ ess \ sup_\Omega |f| & \text{if } p = \infty. \end{cases}$$

where dx is the Lebesgue measure.

Theorem 2.2.1. *For $1 \leq p \leq \infty$, $L^p(\Omega)$ is a Banach space.*

Definition 2.2.3. *A Hilbert space is a Banach space with an inner product.*

Corollary 2.2.1. *The space $L^2(\Omega)$ is a Hilbert space, with*

$$(f, g)_\Omega = \int\limits_\Omega f g dx.$$

Note that in particular $||f|| = \sqrt{(f, f)_\Omega}$

2.3 Sobolev spaces

To understand the concept of Sobolev spaces we first need to properly define weak derivatives. The basic motivation for looking at weak derivatives is that sometimes a PDE does not have a classical solution. This usually is depending on conditions we wish to impose. By moving to a larger framework, namely that of weak solutions, we are capable of finding solutions to the PDE we could not have found otherwise.

Definition 2.3.1. *Any vector* $\alpha = (\alpha_1, ..., \alpha_k) \in \mathbb{N}^m$ *is called a (m-dimensional) multiindex.*
We use multiindex notation for the description of partial derivatives and write

$$D^\alpha f := \frac{D^{|\alpha|} f}{D^{\alpha_1} x_1 ... D^{\alpha_k} x_k},$$

where $|\alpha| = \alpha_1 + ... + \alpha_k$.

Definition 2.3.2. *Suppose* $u, v \in L^1_{loc}(\Omega)$ *(locally summable) and* α *is a multiindex. Then* v *is the* α^{th} *weak partial derivative of* u*, written as*

$$D^\alpha u = v,$$

provided

$$\int_\Omega u D^\alpha \phi dx = (-1)^{|\alpha|} \int_\Omega v \phi dx \tag{2.1}$$

for all test functions $\phi \in C_c^\infty(\Omega)$. *So, given a certain* u*, if there exists a* v *such that (2.1) is satisfied for all test functions* ϕ*, we say that* $D^\alpha u = v$ *in the weak sense.*

Theorem 2.3.1. *A weak* α^{th} *partial derivative of* u*, when existing, is unique up to a zero-measured set.*

Let $1 \leq p \leq \infty$ and $k \geq 0$ an integer. Now we can define function spaces whose members have weak derivatives of various orders lying in various L^p spaces.

Definition 2.3.3. *A Sobolev space* $W^{k,p}(\Omega)$ *consists of the set of all locally summable functions such that for every multiindex* α *with* $|\alpha| \leq k$*, the weak partial derivative* $D^\alpha u$ *belongs to* $L^p(\Omega)$. *If* $u \in W^{k,p}(\Omega)$*, its norm is:*

$$||u||_{W^{k,p}(\Omega)} := \begin{cases} \left(\sum_{|\alpha| \leq k} \int_\Omega |D^\alpha u|^p \, dx \right)^{\frac{1}{p}} & \text{if } 1 \leq p < \infty \\ \sum_{|\alpha| \leq k} ess\ sup_\Omega |D^\alpha u| & \text{if } p = \infty. \end{cases}$$

Theorem 2.3.2. *Assume Ω is bounded and $\partial\Omega$ is C^1. Then there exists a bounded linear operator*

$$T : W^{1,p}(\Omega) \to L^p(\partial\Omega)$$

such that

- $Tu = u|_{\partial\Omega}$ *if* $u \in W^{1,p}(\Omega) \bigcap C(\bar{\Omega})$,
- $\|Tu\|_{L^p(\partial\Omega)} \leq C\|u\|_{W^{1,p}(\Omega)}$

for all $u \in W^{1,p}(\Omega)$, with constant C only depending on p and Ω.

Definition 2.3.4. *We call Tu the trace of u on $\partial\Omega$.*

Theorem 2.3.3. *Assume Ω bounded and $\partial\Omega$ is C^1. Suppose $u \in W^{1,p}(\Omega)$. Then $u \in W_0^{1,p}(\Omega)$ if and only if $Tu = 0$ on $\partial\Omega$.*

If $p = 2$ we write $H^k(\Omega) = W^{k,2}(\Omega)$.

Theorem 2.3.4. *$H^k(\Omega)$ is a Hilbert space. Its inner product is*

$$(u, v) = \sum_{|\alpha|\leq k} \int_\Omega D^\alpha u(x) \cdot D^\alpha v(x) dx.$$

Mainly $H^1(\Omega)$ will appear in the remainder of this thesis, where $\Omega \subset \mathbb{R}^2$ with Lipschitz boundary $\partial\Omega$. The space, its norm and its inner product can be defined by

$$H^1(\Omega) := \left\{u \in L^2(\Omega) \mid \text{the weak derivatives } \partial_j u \text{ exist in } L^2(\Omega),\, j = 1, 2\right\},$$

$$\|u\|^2_{H^1(\Omega)} := \|u\|^2_{L^2(\Omega)} + \sum_{j=1}^{2} \|\partial_j u\|^2_{L^2(\Omega)},$$

$$(u, v)_{H^1(\Omega)} := (u, v)_{L^2(\Omega)} + \sum_{j=1}^{2} \left(\partial_j u, \partial_j v\right)_{L^2(\Omega)}.$$

Definition 2.3.5. $H_0^1(\Omega) = \left\{u \in H^1(\Omega) | Tu = 0 \text{ on } \partial\Omega\right\}$.

Working with equations in Hilbert spaces requires the concept of duality. The dual space of a Hilbert space H is defined as:

Definition 2.3.6. *Let H be a Hilbert space. Its dual is the set of all linear bounded functionals on H and denoted by H^*:*

$$H^* := \{F : H \to \mathbb{R} \mid F \text{ linear and bounded}\},$$

having the norm

$$\|F\|_{H^*} := \sup_{\phi\neq 0, \phi\in H} \frac{| < F, \phi >_{H^*,H} |}{\|\phi\|_H}$$

Remark 2.3.1. *$F(\phi) =< F, \phi >_{H^*,H}$ is the called the duality pairing between H^* and H.*

Theorem 2.3.5. *H^* is a Hilbert space.*

In particular, H^{-1} is the dual space of H^1.

2.4 Bochner spaces

Parabolic equations involve two kinds of variables: time and space. To deal with solutions of parabolic problems, one can fix t and interpret $f(t)$ as an element of a Banach space. This leads to the concept of Bochner spaces.

Definition 2.4.1. *A measurable function $f : \Omega \to B$ is Bochner integrable if there exists a sequence of integrable simple functions s_n such that*

$$\lim_{n\to\infty} \int_\Omega \|f - s_n\|_B d\mu = 0.$$

Here the integral is an ordinary Lebesgue integral. The Bochner integral is now defined by

$$\int_\Omega f d\mu = \lim_{n\to\infty} \int_\Omega s_n d\mu.$$

Definition 2.4.2. *Let $f, g \in L^1(0, T; X)$ where f, g are both Bochner integrable and X is a Banach space. Then $f' = g$ is the Bochner derivative if for all $\phi \in C_0^\infty(0, T)$ holds that*

$$\int_0^T f(t)\phi'(t)dt = -\int_0^T g(t)\phi(t)dt.$$

Definition 2.4.3. *Let X be a Banach space. The following spaces are Bochner spaces:*

$$L^2(0, T; X) := \left\{ f : [0, T] \to X \text{ measurable} \mid \|f\|^2_{L^2(0,T;X)} := \int_0^T \|f(t)\|_X^2 dt < \infty \right\}.$$

$$H^1(0, T; X) := \left\{ f \in L^2(0, T; X) \mid \exists g \in L^2(0, T; X) \text{ such that } f' = g \text{ Bochner derivative} \right\}.$$

If H is a Hilbert space, the following is an inner product on $L^2(0, T; H)$:

$$(f, g)_{L^2(0,T;H)} := \int_0^T (f(t), g(t))_H \, dt$$

Then the Bochner space is also a Hilbert space.

Definition 2.4.4. *The space* $\mathcal{W} = \left\{u \in L^2\left(0, T; H^1(\Omega)\right) | \partial_t u \in L^2\left(0, T; H^{-1}(\Omega)\right)\right\}$.

Remark 2.4.1. *In the case that* $H = L^2(\Omega)$*, we denote*

$$\begin{aligned} (f, g)_{\Omega T} &:= (f, g)_{L^2(0,T;H)}, \\ \|f\|_{\Omega T} &:= \|f\|_{L^2(0,T;H)}. \end{aligned}$$

2.5 (In)equalities

Throughout this thesis, we use the following standard (in)equalities:

Cauchy-Schwarz Inequality
Assume $x, y \in \mathbb{R}^n$. Then

$$|x \cdot y| \le |x|\,|y| \le \frac{\delta}{2}\|x\|^2 + \frac{1}{2\delta}\|y\|^2.$$

Triangle inequality
Suppose $u, v \in X$ where X is a normed space. Then

$$\begin{aligned} ||u+v||_X &\le ||u||_X + ||v||_X, \\ |||u||_X - ||v||_X| &\le ||u-v||_X. \end{aligned}$$

Hölder's inequality
Assume $1 \le p, q \le \infty$, $\frac{1}{p} + \frac{1}{q} = 1$. Then if $u \in L^p(\Omega)$, $v \in L^q(\Omega)$, we have

$$\int_\Omega |uv|\,dx \le ||u||_{L^p(\Omega)}\,||v||_{L^q(\Omega)}.$$

Trace inequality
Assume Ω bounded and $\partial\Omega$ Lipschitz. Then

$$\|u\|^2_{L^2(\partial\Omega)} \le C\left(\|u\|^2_{L^2(\Omega)} + \|u\|_{L^2(\Omega)}\|\nabla u\|_{L^2(\Omega)}\right)$$

for all $u \in H^1(\Omega)$, and C depending on Ω only.

Poincaré's inequality
Assume Ω bounded, open subset of $\mathbb{R}^n$. Suppose $u \in W_0^{1,p}(\Omega)$ for some $1 \le p < n$. Then for all $1 \le p \le \infty$,

$$\|u\|_{L^p(\Omega)} \le c\|Du\|_{L^p(\Omega)}$$

where c depends only on p, n and Ω.

Gronwall's inequality

- Let ξt be a nonnegative summable function on [0,T] which satisfies for a.e. t the following inequality:

$$\xi(t) \leq C_1 \int_0^t \xi(s)ds + C_2$$

where constants $C_1, C_2 \geq 0$. Then

$$\xi(t) \leq C_2 \left(1 + C_1 t e^{C_1 t}\right)$$

for a.e. $0 \leq t \leq T$.

- In particular when

$$\xi(t) \leq C_1 \int_0^t \xi(s)ds$$

for a.e. $0 \leq t \leq T$, then

$$\xi(t) = 0 \text{ a.e.}$$

Identity 1
Let $a, b \in \mathbb{R}$. Then the inner product

$$(a-b, a) = \frac{1}{2}\Big(a^2 + (a-b)^2 - b^2\Big) \tag{2.2}$$

2.6 Important theorems

Theorem 2.6.1 (Dominated convergence theorem)**.**
Assume the functions $\{f_k\}_{k=1}^{\infty}$ are integrable and $f_k \to f$ a.e. for $k \to \infty$.
Suppose also $|f_k| \leq g$ a.e., for some summable function g. Then

$$\int_{\mathbb{R}^n} f_k dx \to \int_{\mathbb{R}^n} f dx.$$

Theorem 2.6.2 (Lax-Milgram Theorem)**.** *Given a Hilbert space H, a continuous, coercive bilinear form $a(\cdot,\cdot)$ $(a : H \times H \to \mathbb{R})$ and a continuous linear functional $F \in H^*$, there exists a unique $u \in H$ such that*

$$a(u, \phi) = F(\phi) \forall \phi \in H.$$

Theorem 2.6.3 (Eberlein-Šmulian)**.**
If X is a Banach space, and $A \subseteq X$ then the following statements are equivalent:

- *Each sequence of elements of A has a subsequence that is weakly convergent.*
- *Each sequence of elements of A has a weak cluster point.*
- *The weak closure of A is weakly compact.*

3 Modeling

In this chapter we will briefly introduce the mathematical model. After that, we turn to the process of making this problem dimensionless, which is very important for gaining insights into our problem. The dimensionless problem not only gives us the relative importance of the model terms and components, it also avoids round-off due to large/small number manipulations. Good examples of normalizing a model can be found in [5].
In this thesis, we will look at the adsorption and desorption model. However, the techniques that we apply here can also be applied to other models, such as for example the precipitation and dissolution model (see [10]). We consider the shape of the geometry to be independent of the concentration of the ions and the solid. This means that Ω as well as Γ do not depend on either the concentration of the dissolved species $\tilde{u}$ or the concentration of the adsorbent $\tilde{v}$. The case where the oscillating boundaries are in fact moving in time due to the influence of reactions, is discussed in [11] and [14].

3.1 Adsorption and desorption model

We consider the bounded domain Ω. This domain is occupied by a fluid containing dissolved cations and anions. Let $\Omega^T = (0, T] \times \Omega$.

We consider a simplified model for the diffusion of the solute, described by the linear diffusion equation. In this equation, we do not take the flow into account. In fact, one can take it into account, but if the chemical processes do not affect the flow parameters on the domain, the flow can be decoupled and hence is seen as given (see e.g. Chapter 3 of [9]).

The linear diffusion equation to describe this model:

$$\partial_{\tilde{t}}\tilde{u} - \tilde{D}\Delta_{\tilde{x}}\tilde{u} = 0 \in \Omega^T. \tag{3.1}$$

The process of adsorption and desorption takes place on boundary $\Gamma \in \partial\Omega$. Let $\Gamma^T = (0, T] \times \Gamma$. Having v the concentration of the adsorbent (a solid) we can write

$$\partial_t v = r_a - r_d \text{ on } \Gamma^T,$$

where r_a and r_d are respectively the adsorption and desorption rate. In our model we will use $r_a = k_a\tilde{u}$ so the adsorption rate is only depending on the concentration of the solute. Furthermore we assume the desorption rate $r_d = k_d\tilde{v}$ is solely depending on the concentration of solid.

On the boundary Γ we have the adsorption/desorption equations

$$-\tilde{D}\partial_{\tilde{\nu}}\tilde{u} = \partial_{\tilde{t}}\tilde{v} \quad (3.2)$$

$$\partial_{\tilde{t}}\tilde{v} = k_a\tilde{u} - k_d\tilde{v} \quad (3.3)$$

where k_a and k_d are respectively the adsorption and desorption rate constants.
In our model we assume both the adsorption rate and desorption rate to be linear depending on the concentrations of respectively the ions and the solid. This is a simplification for a model previously used in [6] and [4].

3.2 Dimensionless model

We will now make equations (3.1) - (3.3) dimensionless, and therefore we need to introduce the appropriate scales. Take $\hat{u}$, $\hat{v}$ as the characteristic concentrations, $\hat{L}$ as the characteristic length, and $\hat{T}$ as the characteristic time. Setting

$$u = \frac{\tilde{u}}{\hat{u}}, v = \frac{\tilde{v}}{\hat{v}}, x = \frac{\tilde{x}}{\hat{L}}, t = \frac{\tilde{t}}{\hat{T}}$$

we find that

$$\partial_{\tilde{t}} = \frac{1}{\hat{T}}\partial_t, \partial_{\tilde{x}} = \frac{1}{\hat{L}}\partial_x$$

and we obtain for (3.1) the following dimensionless equation:

$$\frac{\hat{u}}{\hat{T}}\partial_t u - \frac{\tilde{D}}{\hat{L}^2}\hat{u}\Delta_x u = 0 \text{ in } \Omega.$$

Multiplication with $\frac{\hat{T}}{\hat{u}}$ gives

$$\partial_t u - \frac{\tilde{D}}{\hat{L}^2}\hat{T}\Delta_x u = 0 \text{ in } \Omega,$$

where $\frac{\tilde{D}}{\hat{L}^2}\hat{T}$ is a dimensionless constant D. Taking the diffusion time scale $\hat{T} = \frac{\hat{L}^2}{\tilde{D}}$ we get $D = 1$ leaving the following equation:

$$\partial_t u - \Delta u = 0 \text{ in } \Omega. \quad (3.4)$$

Now we turn to (3.2). We get the following dimensionless equation:

$$-\frac{\tilde{D}}{\hat{L}}\hat{u}\partial_\nu u = \frac{\hat{v}}{\hat{T}}\partial_t v \text{ on } \Gamma.$$

Since $\tilde{D} = \frac{\hat{L}^2}{\hat{T}}$ (so $D = 1$) we get

$$-\partial_\nu u = \frac{1}{\hat{L}}\frac{\hat{v}}{\hat{u}}\partial_t v \text{ on } \Gamma.$$

We can make an assumption for both $\hat{v}$ and $\hat{u}$. Therefore we introduce the reference situation where $\tilde{u} = \hat{u}$ everywhere in Ω and $\tilde{v} = \hat{v}$ everywhere on Γ. Assuming the weights of $\tilde{u}$ and $\tilde{v}$ the same in this reference situation, it follows that a natural assumption is that $\hat{v} = \hat{L}\hat{u}$. We end up with

$$-\partial_\nu u = \partial_t v \text{ on } \Gamma. \tag{3.5}$$

For (3.3) we get the following dimensionless equation:

$$\frac{\hat{v}}{\hat{T}}\partial_t v = k_a\hat{u}u - k_d\hat{v}v \text{ on } \Gamma.$$

Using the earlier assumption that $\hat{v} = \hat{L}\hat{u}$ we get

$$\begin{aligned}\partial_t v &= \frac{\hat{T}}{\hat{L}}k_a u - \hat{T}k_d v \\ &= \hat{T}k_d\left(\frac{k_a}{\hat{L}k_d}u - v\right) \text{ on } \Gamma.\end{aligned}$$

Now assume $k_a \sim \hat{L}k_d$ and define $k := \frac{k_a}{\hat{L}k_d}$. Furthermore $Da = \hat{T}k_d$ is the Damkohler number. We end up with

$$\partial_t v = Da\,(ku - v) \text{ on } \Gamma. \tag{3.6}$$

Equations (3.4), (3.5) and (3.6) give us the dimensionless form of the problem.
Alternative scalings are considered in [12] or [5].

4 Rothe's method

4.1 Introduction

Before using Rothe's method to prove existence of weak solutions to our problem, we first state how the method works. The idea is to discretize both u and v in time for some step size τ. We then proceed to acquiring τ-independent bounds for the time-discrete series u^n and v^n, after showing that these series exist. The next step is to use time-dependent piecewise linear approximations U^τ and V^τ where the interpolation points are supplied by the time-discrete series. We will try to use the bounds from the time-discrete series to get bounds for these approximations. We use compactness arguments to get existence of the limits of these approximations as $\tau \searrow 0$. Then we show that the limits solve the parabolic problem. Then finally we show that this solution is also unique.
Existence results for similar problems, but in a perforated domain, are obtained in e.g. [8] The problem is given formally as:

Problem 4.1.1. *Find u, v such that*

$$\begin{cases} \partial_t u - \triangle u &= 0 & \text{in } \Omega \times (0,T) \\ u &= u_I & \text{in } \Omega \text{ for } t = 0 \\ u &= 0 & \text{on } (\partial\Omega / \Gamma) \times (0,T) \\ \overrightarrow{n} \cdot \nabla u &= -\partial_t v & \text{on } \Gamma \times (0,T) \\ \partial_t v &= Da\,(ku - v) & \text{on } \Gamma \times (0,T) \\ v &= v_I & \text{on } \Gamma \text{ for } t = 0 \end{cases} \tag{4.1}$$

In general, the boundary condition $u = u_D$ where $u_D \in L^2\left(0, T; H^1(\Omega)\right)$ can be reduced to the case where $u_D = 0$ by simply subtracting u_D from u everywhere in domain Ω. Also Robin type boundary conditions can be considered.
Figure 4.1 is a visualization of the situation. In general, we will not be able to find a classical solution for Problem 4.1.1. Therefore we have to turn to the following variational problem:

Definition 4.1.1. *Find $u \in L^2\left(0, T; H^1(\Omega)\right)$, $v \in H^1\left(0, T; L^2(\Gamma)\right)$ such that $u(0,\cdot) = u_I$ and $\partial_t u \in L^2\left(0, T; H^{-1}(\Omega)\right)$ and for all $\phi \in L^2\left(0, T; H^1(\Omega)\right)$ and $\theta \in L^2\left(0, T; L^2(\Gamma)\right)$ it*

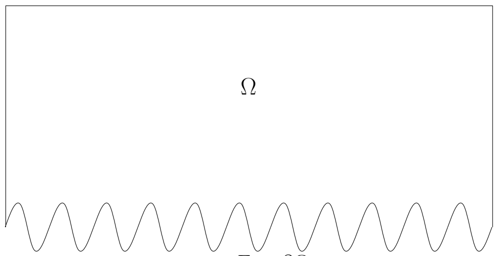

Figure 4.1: A sketch of the domain and its boundaries.

holds that

$$\begin{aligned}(\partial_t u, \phi)_\Omega + (\nabla u, \nabla \phi)_\Omega &+ (\partial_t v, \phi)_\Gamma = 0, \\ (\partial_t v, \theta)_\Gamma &= (Da\,(ku - v)\,, \theta)_\Gamma\,,\end{aligned}$$

for all $\phi, \theta \in H^1(\Omega)$.

4.2 Time discretization

First we discretize time, using the implicit Euler method for u and the explicit Euler method for v. Let T be the final time, and divide the interval $[0, T]$ in N equal time steps. Then we define $\tau := \frac{T}{N}$ the size of a time step. On interpolation times $t^n := n\tau$ we can now construct sequences $\{u^n\}_{n=1}^N$ and $\{v^n\}_{n=1}^N$, that are weak solutions of the following system of partial differential equations:

$$\begin{aligned}\frac{u^n - u^{n-1}}{\tau} - \triangle u^n &= 0 \text{ in } \Omega \times (0, T) \\ \overrightarrow{n} \cdot \nabla u^n &= -\frac{v^n - v^{n-1}}{\tau} \text{ on } \Gamma \times (0, T) \\ \frac{v^n - v^{n-1}}{\tau} &= Da\left(ku^n - v^{n-1}\right) \text{ on } \Gamma \times (0, T)\end{aligned}$$

Definition 4.2.1. *We define*

$$H^1_{0,\Gamma}(\Omega) := \left\{u \in H^1(\Omega) | Tu = 0 \text{ on } \partial\Omega / \Gamma\right\},$$

where Tu *is defined as in Theorem 2.3.2.*

A more appropriate form of this system of equations is given by:

Definition 4.2.2. *Let u^{n-1}, v^{n-1} be given. A pair $(u^n, v^n) \in H^1_{0,\Gamma}(\Omega) \times L^2(\Gamma)$ is called a weak solution if*

$$\left(\frac{u^n - u^{n-1}}{\tau}, \phi\right)_\Omega + \left(\nabla u^n, \nabla\phi\right)_\Omega + \left(\frac{v^n - v^{n-1}}{\tau}, \phi\right)_\Gamma = 0, \tag{4.2}$$

$$\left(\frac{v^n - v^{n-1}}{\tau}, \theta\right)_\Gamma = \left(Da\left(ku^n - v^{n-1}\right), \theta\right)_\Gamma, \tag{4.3}$$

for all $\phi, \theta \in H^1(\Omega)$.

4.3 Existence and uniqueness of the time discrete problem

Formally, u^n and v^n satisfy

$$u^n - \tau\Delta u^n = u^{n-1} \text{ in } \Omega \tag{4.4}$$

$$-\tau\overrightarrow{n}\nabla u^n = Da\left(ku^n - v^{n-1}\right) \text{ on } \Gamma \tag{4.5}$$

$$v^n = v^{n-1} + \tau Da\left(ku^n - v^{n-1}\right) \text{ on } \Gamma \tag{4.6}$$

This means that for a given u^{n-1} and v^{n-1} we can determine u^n independently of v^n. We can obtain existence and uniqueness of the latter directly by showing existence and uniqueness for u^n. To this aim we introduce the weak form of (4.4) - (4.6), and use the Lax-Milgram theorem.

From equations (4.2) and (4.3) we can conclude that a solution pair (u^n, v^n) satisfies

$$\left(\nabla u^n, \nabla\phi\right)_\Omega + \frac{1}{\tau}\left(u^n, \phi\right)_\Omega + Da\ k\left(u^n, \phi\right)_\Gamma = \frac{1}{\tau}\left(u^{n-1}, \phi\right)_\Omega + Da\left(v^{n-1}, \phi\right)_\Gamma$$

for all $\phi \in H^1_{0,\Gamma}(\Omega)$.
We now use the Lax-Milgram theorem (see Theorem 2.6.2). For this we take

- $H = H^1_{0,\Gamma}(\Omega)$, with $\|u\|_H = \|u\|_{H^1}$,
- $a : H \times H \to \mathbb{R}$,
  $a\left(u^n, \phi\right) = \left(\nabla u^n, \nabla\phi\right)_\Omega + \frac{1}{\tau}\left(u^n, \phi\right)_\Omega + Da\ k\left(u^n, \phi\right)_\Gamma$,
- $F : H \to \mathbb{R}$,
  $F(\phi) = \frac{1}{\tau}\left(u^{n-1}, \phi\right)_\Omega + Da\left(v^{n-1}, \phi\right)_\Gamma$.

We remark that in this case H is in fact a Hilbert space.
Bilinearity of $a\left(u^n, \phi\right)$ and linearity of $F(\phi)$ is straightforward.

We have to show that $a(u^n, \phi)$ is continuous and coercive, and that $F(\phi)$ is continuous. Every continuous function from a compact space into a metric space is bounded, so it is sufficient to show both $a(u^n, \phi)$ and $F(\phi)$ are bounded.

Lemma 4.3.1. $a(u^n, \phi)$ *is coercive.*

Proof. We have to show that $\exists c > 0 : a(u^n, u^n) \geq c\|u^n\|_H^2 \forall u^n \in H$. Let $u^n \in H$. Now

$$\begin{aligned} a\left(u^n, u^n\right) &= \left(\nabla u^n, \nabla u^n\right)_\Omega + \frac{1}{\tau}\left(u^n, u^n\right)_\Omega + Da\ k\left(u^n, u^n\right)_\Gamma \\ &\geq \left(\nabla u^n, \nabla u^n\right)_\Omega + \frac{1}{\tau}\left(u^n, u^n\right)_\Omega \\ &= \|\nabla u^n\|_\Omega^2 + \frac{1}{\tau}\|u^n\|_\Omega^2 \\ &\geq \min\left(1, \frac{1}{\tau}\right)\|u^n\|_H^2 \quad \square \end{aligned}$$

Lemma 4.3.2. $a(u^n, \phi)$ *is bounded.*

Proof. We have to show that $\exists c > 0 : a(u^n, u^n) \leq c\|u^n\|_H\|\phi\|_H \forall u^n, \phi \in H$. Let $u^n, \phi \in H$. Now

$$\begin{aligned} a\left(u^n, \phi\right) &= \left(\nabla u^n, \nabla \phi\right)_\Omega + \frac{1}{\tau}\left(u^n, \phi\right)_\Omega + Da\ k\left(u^n, \phi\right)_\Gamma \\ &\leq \|\nabla u^n\|_\Omega\|\nabla\phi\|_\Omega + \frac{1}{\tau}\|u^n\|_\Omega\|\phi\|_\Omega + Da\ k\|u^n\|_\Gamma\|\phi\|_\Gamma \\ &\leq \|\nabla u^n\|_\Omega\|\nabla\phi\|_\Omega + \frac{1}{\tau}\|u^n\|_\Omega\|\phi\|_\Omega + Da\ k\|u^n\|_\Omega\|\phi\|_\Omega \\ &\leq \left(1 + \frac{1}{\tau} + Da\ k\right)\|u^n\|_H\|\phi\|_H \quad \square \end{aligned}$$

Lemma 4.3.3. $F(\phi)$ *is bounded.*

Proof. We have to show that $\exists c > 0 : F(\phi) \leq c\|\phi\|_H \forall \phi \in H$. Let $\phi \in H$. Now

$$\begin{aligned} F(\phi) &= \frac{1}{\tau}\left(u^{n-1}, \phi\right)_\Omega + Da\left(v^{n-1}, \phi\right)_\Gamma \\ &\leq \frac{1}{\tau}\|u^{n-1}\|_\Omega\|\phi\|_\Omega + Da\|v^{n-1}\|_\Gamma\|\phi\|_\Gamma \\ &\leq \left(\frac{1}{\tau}\|u^{n-1}\|_\Omega\| + Da\|v^{n-1}\|_\Gamma\right)\|\phi\|_H \quad \square \end{aligned}$$

Lemmas 4.3.1 - 4.3.3 show that all requirements for the Lax-Milgram lemma are fulfilled. Hence there exists a unique $u^n \in H^1_{0,\Gamma}$. Furthermore, we can obtain existence and uniqueness of v^n directly by using Equation (4.6).

4.4 A priori estimates

Having obtained the existence and uniqueness of a solution of the time discrete problems, we proceed by giving a priori estimates. First we need the following essential L^∞-bounds:

Lemma 4.4.1. *Assume $\tau < \frac{1}{Da}$ and u^{n-1} and v^{n-1} are nonnegative. Then u^n and v^n are nonnegative as well.*

Proof. Testing with $\phi := \left[u^n\right]_-$ (the non-positive part of u^n) in Ω using equation (4.2) gives us

$$\begin{aligned}\left(\nabla u^n, \nabla \left[u^n\right]_-\right)_\Omega + \frac{1}{\tau}\left(u^n, \left[u^n\right]_-\right)_\Omega &+ Da\ k\left(u^n, \left[u^n\right]_-\right)_\Gamma \\ &= \frac{1}{\tau}\left(u^{n-1}, \left[u^n\right]_-\right)_\Omega + Da\left(v^{n-1}, \left[u^n\right]_-\right)_\Gamma\end{aligned}$$

which leads to

$$\tau \| \nabla \left[u^n\right]_- \|_\Omega^2 + \| \left[u^n\right]_- \|_\Omega^2 + Da\ k\tau \| \left[u^n\right]_- \|_\Gamma^2 = \left(u^{n-1}, \left[u^n\right]_-\right)_\Omega + Da\left(v^{n-1}, \left[u^n\right]_-\right)_\Gamma$$

All terms on the left hand side are nonnegative, where the terms on the right are non-positive as both u^{n-1} and $v^{n-1} \geq 0$. We obtain that $\left[u^n\right]_- = 0$ and therefore u^n is nonnegative.
Test with $\theta := \left[v^n\right]_-$ (the non-positive part of v^n) on Γ using equation (4.3) to obtain:

$$\| \left[v^n\right]_- \|_\Gamma^2 = Da\ \tau k\left(u^n, \left[v^n\right]_-\right)_\Gamma + (1 - Da\ \tau)\left(v^{n-1}, \left[v^n\right]_-\right)$$

Because of the assumptions on τ and v^{n-1} and the previous result on u^n, all terms on the right hand side are nonpositive, which leads ultimately to

$$\| \left[v^n\right]_- \|_\Gamma^2 \leq 0,$$

showing v^n is nonnegative. □

Lemma 4.4.2. *Assume $\tau < \frac{1}{Da}$. Let $M \in \mathbb{R}$ such that $u^{n-1} \leq M$ and $v^{n-1} \leq kM$. Then $u^n \leq M$ and $v^n \leq kM$.*

Proof. Testing with $\phi := \left[u^n - M\right]_+$ (the nonnegative part of $u^n - M$) in Ω using equation (4.2) gives us

$$\begin{aligned}\left(\nabla u^n, \nabla \left[u^n - M\right]_+\right)_\Omega &+ \frac{1}{\tau}\left(u^n - M, \left[u^n - M\right]_+\right)_\Omega + Da\ k\left(u^n - M, \left[u^n - M\right]_+\right)_\Gamma \\ &= \frac{1}{\tau}\left(u^{n-1} - M, \left[u^n - M\right]_+\right)_\Omega + Da\left(v^{n-1} - kM, \left[u^n - M\right]_+\right)_\Gamma\end{aligned}$$

which leads to

$$\begin{aligned}\tau\|\nabla\left[u^n-M\right]_+\|_\Omega^2 \;&+\; \|\left[u^n-M\right]_+\|_\Omega^2+Da\ \tau k\|\left[u^n-M\right]_+\|_\Gamma^2\\ &=\; \left(u^{n-1}-M,\left[u^n-M\right]_+\right)_\Omega+Da\ \tau\left(v^{n-1}-kM,\left[u^n-M\right]_+\right)_\Gamma\end{aligned}$$

Since $u^{n-1}\le M$ and $v^{n-1}\le kM$ all the terms on the right hand side are nonpositive. Because all the terms on the left hand side are nonnegative it follows that $u^n\le M$. Testing with $\theta:=\left[v^n-kM\right]_+$ on Γ using equation (4.3) gives us that

$$\|\left[v^n-kM\right]_+\|_\Gamma^2=Da\ \tau k\left(u^n-M,\left[v^n-kM\right]_+\right)_\Gamma+(1-Da\ \tau)\left(v^{n-1}-kM,\left[v^n-kM\right]_+\right)$$

Since $\tau<1, v^{n-1}\le kM$ and $u^n\le M$, we find that the right hand side consists of nonpositive terms only, while the left hand side is nonnegative. This gives us $v^n\le kM$. □

With initial values u_I and v_I and the Dirichlet boundary condition $u_D=0$ on $(\partial\Omega\ /\ \Gamma)$ we can conclude that

$$M=\max\left\{0,||u_I||_{L^\infty(\Omega)},\frac{1}{k}\,||v_I||_{L^\infty(\Gamma)}\right\}.$$

The L^∞ estimates immediately lead to:

Lemma 4.4.3. *There exists a $C>0$ such that for any $n\in\{1,...,N\}$ one has*

$$\|v^n\|_\Gamma+\|u^n\|_\Gamma+\|u^n\|_\Omega\le C. \tag{4.7}$$

Now we obtain energy estimates. We start with

Lemma 4.4.4. *A $C>0$ exists such that for any $n\in\{1,...,N\}$ it holds that $\|v^n-v^{n-1}\|_\Gamma\le C\tau$.*

Proof. Testing with $\theta=v^n-v^{n-1}$ gives

$$\begin{aligned}\left(v^n-v^{n-1},v^n-v^{n-1}\right)_\Gamma &= Da\ \tau\left(ku^n-v^{n-1},v^n-v^{n-1}\right)_\Gamma\\ \|v^n-v^{n-1}\|_\Gamma^2 &\le Da\ \tau\|ku^n-v^{n-1}\|_\Gamma\|v^n-v^{n-1}\|_\Gamma\\ \|v^n-v^{n-1}\|_\Gamma &\le Da\ \tau\left(k\|u^n\|_\Gamma+\|v^{n-1}\|_\Gamma\right)\\ \|v^n-v^{n-1}\|_\Gamma &\le C\tau\end{aligned}$$

where the last step is justified because of the earlier shown boundedness of both sequences u^n and v^n.

□

Similarly, for u one has:

Lemma 4.4.5. *There exists a $C > 0$ such that*

$$\tau \sum_{n=1}^{N} \|\nabla u^n\|_\Omega^2 + \sum_{n=1}^{N} \|u^n - u^{n-1}\|_\Omega^2 + \tau \sum_{n=1}^{N} \|\nabla \left(u^n - u^{n-1}\right)\|_\Omega^2 + \sum_{n=1}^{N} \|u^n - u^{n-1}\|_\Gamma^2 \leq C.$$

Proof. Testing with $\phi = u^n$ gives

$$\left(u^n - u^{n-1}, u^n\right)_\Omega + \tau \left(\nabla u^n, \nabla u^n\right)_\Omega + Da\ \tau \left(ku^n - v^{n-1}, u^n\right)_\Gamma = 0$$

Using the identity given by (2.2) we get

$$\frac{1}{2}\left(\|u^n\|_\Omega^2 - \|u^{n-1}\|_\Omega^2 + \|u^n - u^{n-1}\|_\Omega^2\right) + \tau\|\nabla u^n\|_\Omega^2 + Da\ \tau k\|u^n\|_\Gamma^2 \leq Da\ \left(\frac{1}{2}\tau\|v^{n-1}\|_\Gamma^2 + \frac{1}{2}\tau\|u^n\|_\Gamma^2\right)$$

Summing over $n = 1$ to $n = N$ and using the bound (4.7) gives

$$\begin{aligned} \frac{1}{2}\|u^N\|_\Omega^2 + \frac{1}{2}\sum_{n=1}^{N}\|u^n - u^{n-1}\|_\Omega^2 &+ \tau\sum_{n=1}^{N}\|\nabla u^n\|_\Omega^2 + \tau\sum_{n=1}^{N} Da\ k\|u^n\|_\Gamma^2 \\ &\leq \frac{1}{2}\|u_I\|_\Omega^2 + \tau Da\ \sum_{n=1}^{N} c \leq C \end{aligned} \tag{4.8}$$

Testing with $\phi = u^n - u^{n-1}$ gives

$$\left(u^n - u^{n-1}, u^n - u^{n-1}\right)_\Omega + \tau\left(\nabla u^n, \nabla u^n - \nabla u^{n-1}\right)_\Omega + Da\ \tau\left(ku^n - v^{n-1}, u^n - u^{n-1}\right)_\Gamma = 0$$

Using the identity given by (2.2) twice, we get

$$\begin{aligned} \|u^n - u^{n-1}\|_\Omega^2 &+ \frac{\tau}{2}\left(\|\nabla u^n\|_\Omega^2 - \|\nabla u^{n-1}\|_\Omega^2 + \|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2\right) \\ &+ \frac{Da\ \tau k}{2}\left(\|u^n\|_\Gamma^2 + \|u^n - u^{n-1}\|_\Gamma^2 - \|u^{n-1}\|_\Gamma^2\right)_\Gamma - Da\ \tau\left(v^{n-1}, u^n - u^{n-1}\right)_\Gamma. \end{aligned}$$

With

$$\tau\left(v^{n-1}, u^n - u^{n-1}\right)_\Gamma \leq \frac{k\tau}{4}\|u^n - u^{n-1}\|_\Gamma^2 + \frac{\tau}{4k}\|v^{n-1}\|_\Gamma^2$$

this gives

$$\begin{aligned} \|u^n - u^{n-1}\|_\Omega^2 &+ \frac{\tau}{2}\left(\|\nabla u^n\|_\Omega^2 - \|\nabla u^{n-1}\|_\Omega^2 + \|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2\right) \\ &+ \frac{Da\ \tau k}{2}\left(\|u^n\|_\Gamma^2 - \|u^{n-1}\|_\Gamma^2 + \frac{1}{2}\|u^n - u^{n-1}\|_\Gamma^2\right) = \frac{Da\ \tau}{4k}\|v^{n-1}\|_\Gamma^2 \end{aligned}$$

Summing over $n = 1$ to $n = N$ gives

$$\begin{aligned}\frac{\tau}{2}\|\nabla u^N\|_\Omega^2 &+ \frac{\tau}{2}\sum_{n=1}^{N}\|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2 + \sum_{n=1}^{N}\|u^n - u^{n-1}\|_\Omega^2 + \frac{Da\ \tau k}{2}\|u^N\|_\Gamma^2 \\ &+ \frac{Da\ \tau k}{4}\sum_{n=1}^{N}\|u^n - u^{n-1}\|_\Gamma^2 \le \frac{\tau}{2}\|\nabla u_I\|_\Omega^2 + \frac{Da\ \tau k}{2}\|u_I\|_\Gamma^2 \\ &+ \frac{Da\ \tau}{4k}\sum_{n=1}^{N}\|v^{n-1}\|_\Gamma^2 \le C\tau \end{aligned} \tag{4.9}$$

From estimates 4.8 and 4.9 we conclude that:

$$\begin{aligned}\sum_{n=1}^{N}\|u^n - u^{n-1}\|_\Omega^2 &+ \sum_{n=1}^{N}\|u^n - u^{n-1}\|_\Gamma^2 \\ &+ \tau\left(\sum_{n=1}^{N}\|\nabla u^n\|_\Omega^2 + \sum_{n=1}^{N}\|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2\right) \le C \quad \square \end{aligned} \tag{4.10}$$

4.5 Interpolation in time

We have analyzed the sequence of time-discrete solutions. Using interpolation, we construct a piecewise linear solution approximation for a.e. $t \in [0, T]$. For any $n = 1, 2, ..., N$ and $t \in \left(t^{n-1}, t^n\right]$ we define

$$\begin{aligned} U^\tau &= u^{n-1} + \frac{t - t^{n-1}}{\tau}\left(u^n - u^{n-1}\right), \\ V^\tau &= v^{n-1} + \frac{t - t^{n-1}}{\tau}\left(v^n - v^{n-1}\right). \end{aligned}$$

For these time continuous U^τ and V^τ we can use the bounds and estimates from section 4.4 to derive:

Lemma 4.5.1. *For all $\tau > 0, \tau < \frac{1}{Da}$ the following holds:*

$$0 \le U^\tau \le M \qquad \text{a.e. in } \Omega^T, \tag{4.11}$$

$$0 \le V^\tau \le kM \qquad \text{a.e. on } \Gamma^T, \tag{4.12}$$

$$\|U^\tau(t)\|_\Omega^2 + \|V^\tau(t)\|_\Gamma^2 \le C \quad \text{for all } 0 \le t \le T, \tag{4.13}$$

$$\|\partial_t U^\tau\|_{L^2(0,T;H^{-1}(\Omega))}^2 + \|\nabla U^\tau\|_{\Omega^T}^2 + \|\partial_t V^\tau\|_{\Gamma^T}^2 \le C. \tag{4.14}$$

where C does not depend on τ.

Proof. Equations (4.11) and (4.12) follow directly from Theorem 4.4.1 and Theorem 4.4.2. These bounds do not change by using interpolation.
Equation (4.13) is a consequence of estimate (4.10) and of the uniform bounds on v^n.
For equation 4.14 we use

$$\begin{aligned}
\partial_t U^\tau &= \frac{u^n - u^{n-1}}{\tau} \\
\partial_t V^\tau &= \frac{v^n - v^{n-1}}{\tau} \\
\nabla U^\tau &= \frac{t - t^{n-1}}{\tau}\left(\nabla u^n - \nabla u^{n-1}\right)
\end{aligned}$$

For $\partial_t V^\tau$ we get the estimate

$$\int_0^T \|\partial_t V^\tau\|_\Gamma^2 dt = \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|\frac{v^n - v^{n-1}}{\tau}\|_\Gamma^2 dt \leq CN\tau \leq CT.$$

The estimate on ∇U^τ can be made as follows:

$$\begin{aligned}
\int_0^T \|\nabla U^\tau(t)\|_\Omega^2 dt &\leq 2\sum_{n=1}^N \tau\|\nabla u^{n-1}\|_\Omega^2 + \int_{t^{n-1}}^{t^n} 2\frac{\left(t - t^{n-1}\right)^2}{\tau^2}\|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2 dt \\
&\leq 2\tau\sum_{n=1}^N \|\nabla u^{n-1}\|_\Omega^2 + \frac{2\tau}{3}\sum_{n=1}^N \|\nabla\left(u^n - u^{n-1}\right)\|_\Omega^2 dt \leq C
\end{aligned}$$

The estimate for $\|\partial_t U^\tau\|$ follows:

$$\begin{aligned}
\int_0^T \|\partial_t U^\tau\|_{H^{-1}(\Omega)}^2 dt &= \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|\frac{u^n - u^{n-1}}{\tau}\|_\Omega^2 dt \\
&\leq \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|\Delta u^n\|_\Omega^2 dt \\
&= \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \|\nabla\cdot\left(\nabla u^n\right)\|_\Omega^2 dt \leq C
\end{aligned}$$

where we used the previous estimate. □

Having these estimates, we can let $\tau \searrow 0$. Compactness arguments give the existence of (u,v) and a subsequence $\tau \searrow 0$ such that

$$\begin{aligned} U^\tau &\rightharpoonup u \quad \text{weakly in} \quad L^2\Big((0,T);H^1(\Omega)\Big),\\ \partial_t U^\tau &\rightharpoonup \partial_t u \quad \text{weakly in} \quad L^2\Big((0,T);H^{-1}(\Omega)\Big),\\ V^\tau &\rightharpoonup v \quad \text{weakly in} \quad L^2\Big((0,T);L^2(\Gamma)\Big),\\ \partial_t V^\tau &\rightharpoonup \partial_t v \quad \text{weakly in} \quad L^2\Big((0,T);L^2(\Gamma)\Big), \end{aligned}$$

It remains to show that these limits solves the problem (4.1.1) weakly.
Note that for a.e. $t \in \left(t^{n-1}, t^n\right)$:

$$\begin{aligned} \left\langle \partial_t U^\tau, \phi \right\rangle_{H^{-1},H_0^1} + \left(\nabla U^\tau, \nabla\phi\right)_\Omega + \left(\partial_t V^\tau, \phi\right)_\Gamma &= \left(\nabla\left(U^\tau - u^n\right), \nabla\phi\right)_\Omega,\\ \left(\partial_t V^\tau, \theta\right)_\Gamma = Da\Big(k\left(U^\tau,\theta\right)_\Gamma - \left(V^\tau,\theta\right)_\Gamma - k\left(U^\tau - u^n,\theta\right)_\Gamma &+ \Big(V^\tau - v^{n-1},\theta\Big)_\Gamma\Big). \end{aligned}$$

Now we will look more closely what happens along a sequence $\tau \to 0$. First, we integrate over time:

$$\begin{aligned} \int_0^T \left\langle \partial_t U^\tau, \phi \right\rangle_{H^{-1},H_0^1} dt \quad &+ \quad \int_0^T \left(\nabla U^\tau, \nabla\phi\right)_\Omega dt + \int_0^T \left(\partial_t V^\tau, \phi\right)_\Gamma dt\\ &= \quad \int_0^T \left(\nabla\left(U^\tau - u^n\right), \nabla\phi\right)_\Omega dt,\\ \int_0^T \left(\partial_t V^\tau, \theta\right)_\Gamma dt \quad &= \quad Da\left(k\int_0^T \left(U^\tau,\theta\right)_\Gamma dt - \int_0^T \left(V^\tau,\theta\right)_\Gamma dt\right)\\ &\qquad -Da\left(k\int_0^T \left(U^\tau - u^n,\theta\right)_\Gamma dt - \int_0^T \left(V^\tau - v^n,\theta\right)_\Gamma dt\right). \end{aligned}$$

Weak convergence gives us that

$$\begin{aligned}
\int_0^T \left\langle \partial_t U^\tau, \phi \right\rangle_{H^{-1},H_0^1} dt &\to \int_0^T (\partial_t u, \phi)_{H^{-1},H_0^1} dt, \\
\int_0^T \left(\nabla U^\tau, \nabla\phi\right)_\Omega dt &\to \int_0^T (\nabla u, \nabla\phi)_\Omega dt, \\
\int_0^T \left(\partial_t V^\tau, \phi\right)_\Gamma dt &\to \int_0^T (\partial_t v, \phi)_\Gamma dt, \\
\int_0^T \left(U^\tau, \theta\right)_\Gamma dt &\to \int_0^T (u, \theta)_\Gamma dt, \\
\int_0^T \left(V^\tau, \theta\right)_\Gamma dt &\to \int_0^T (v, \theta)_\Gamma dt.
\end{aligned}$$

Furthermore,

$$\begin{aligned}
\left| \int_0^T \left(\nabla\left(U^\tau - u^n\right), \nabla\phi\right)_\Omega dt \right| &= \left| \sum_{n=1}^N \int_{t^{n-1}}^{t^n} \left(\nabla\left(U^\tau - u^n\right), \nabla\phi\right) dt \right| \\
&\le \left(\sum_{n=1}^N \int_{t^{n-1}}^{t^n} \left|\left|\nabla\left(U^\tau - u^n\right)\right|\right|^2 dt \right)^{\frac{1}{2}} \left(\sum_{k=1}^N \int_{t^{n-1}}^{t^n} ||\nabla\phi||^2 dt \right)^{\frac{1}{2}} \\
&= ||\nabla\phi||_{L^2(0,T;L^2(\Omega))} \left(\sum_{n=1}^N \int_{t^{n-1}}^{t^n} \frac{(t^n - t)^2}{\tau^2} \left|\left|\nabla\left(u^n - u^{n-1}\right)\right|\right|^2 dt \right)^{\frac{1}{2}} \\
&\le ||\nabla\phi||_{L^2(0,T;L^2(\Omega))} \, \tau^{\frac{1}{2}} \left(\sum_{n=1}^N \left|\left|\nabla\left(u^n - u^{n-1}\right)\right|\right|^2 \right)^{\frac{1}{2}} \\
&\to 0 \text{ as } \tau \to 0
\end{aligned}$$

and similarly we get that

$$
\begin{aligned}
\left|\int_0^T \left(U^\tau - u^n, \phi\right)_\Gamma dt\right| &= \left|\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \left(U^\tau - u^n, \phi\right)_\Gamma dt\right| \\
&\leq \left(\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \left|\left|U^\tau - u^n\right|\right|^2 dt\right)_\Gamma^{\frac{1}{2}} \left(\sum_{k=1}^{N}\int_{t^{n-1}}^{t^n} ||\phi||_\Gamma^2\, dt\right)^{\frac{1}{2}} \\
&= ||\phi||_{L^2(0,T;L^2(\Gamma))} \left(\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \frac{(t^n - t)^2}{\tau^2} \left|\left|u^n - u^{n-1}\right|\right|_\Gamma^2 dt\right)^{\frac{1}{2}} \\
&\leq ||\phi||_{L^2(0,T;L^2(\Gamma))}\, \tau^{\frac{1}{2}} \left(\sum_{n=1}^{N} \left|\left|u^n - u^{n-1}\right|\right|_\Gamma^2\right)^{\frac{1}{2}} \\
&\to 0 \text{ as } \tau \to 0
\end{aligned}
$$

in view of Lemma 4.4.5. Note that there exists a $C \in \mathbb{R}$ such that

$$||\phi||_{L^2(0,T;L^2(\Gamma))} \leq C\, ||\phi||_{L^2(0,T;H^1(\Omega))}\,.$$

Furthermore,

$$
\begin{aligned}
\left|\int_0^T \left(V^\tau - v^{n-1}, \phi\right)_\Gamma dt\right| &= \left|\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \left(V^\tau - v^{n-1}, \phi\right)_\Gamma dt\right| \\
&\leq \left(\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \left|\left|V^\tau - v^{n-1}\right|\right|_\Gamma^2 dt\right)^{\frac{1}{2}} \left(\sum_{k=1}^{N}\int_{t^{n-1}}^{t^n} ||\phi||_\Gamma^2\, dt\right)^{\frac{1}{2}} \\
&= ||\phi||_{L^2(0,T;L^2(\Gamma))} \left(\sum_{n=1}^{N}\int_{t^{n-1}}^{t^n} \frac{\left(t - t^{n-1}\right)^2}{\tau^2} \left|\left|v^n - v^{n-1}\right|\right|_\Gamma^2 dt\right)^{\frac{1}{2}} \\
&\leq ||\phi||_{L^2(0,T;L^2(\Gamma))}\, \tau^{\frac{1}{2}} \left(\sum_{n=1}^{N} \left|\left|v^n - v^{n-1}\right|\right|_\Gamma^2\right)^{\frac{1}{2}} \\
&\to 0 \text{ as } \tau \to 0
\end{aligned}
$$

in view of Lemma 4.4.4. In this way we have actually proved

Theorem 4.5.1. *Problem 4.1.1 has a weak solution (u, v) in the sense of Definition 4.1.1.*

4.6 Uniqueness of the solution

Having proved existence of the solution in the previous section, we proceed with proving uniqueness.
Suppose we have both (u_1, v_1) and $(u_2, v_2) \in \left(L^2\left((0,T); H^1(\Omega)\right), L^2\left((0,T); L^2(\Gamma)\right)\right)$ solving problem (4.1.1) in the sense of weak solutions and take $u := u_1 - u_2$, $v := v_1 - v_2$.

Clearly (u, v) satisfies

$$\begin{aligned}
(\partial_t u, \phi)_\Omega + (\nabla u, \nabla \phi)_\Omega + (\partial_t v, \phi)_\Gamma &= 0 \\
(\partial_t v, \theta)_\Gamma &= Da\,(ku - v, \theta)_\Gamma \\
u(t=0) &= 0 \text{ in } \Omega \\
v(t=0) &= 0 \text{ on } \Gamma
\end{aligned}$$

for all $\phi \in L^2\left(0, T; H^1(\Omega)\right)$ and $\theta \in L^2\left(0, T; L^2(\Gamma)\right)$ so we will get $u(t) = 0$ a.e. in Ω and $v(t) = 0$ a.e. in Γ.
Take $\theta = v$ to obtain

$$\begin{aligned}
\frac{d}{dt}\|v\|_\Gamma^2 &\leq Da\left(k\|u\|_\Gamma\|v\|_\Gamma + \|v\|_\Gamma^2\right) \\
2\|v\|_\Gamma\frac{d\|v\|_\Gamma}{dt} &\leq Da\left(k\|u\|_\Gamma + \|v\|_\Gamma\right)\|v\|_\Gamma \\
\frac{d\|v\|_\Gamma}{dt} &\leq \frac{Da}{2}k\|u\|_\Gamma + \frac{Da}{2}\|v\|_\Gamma \\
\|v\|_\Gamma &\leq \int_0^t \frac{2}{Da}\left(e^{\frac{Da}{2}s} - 1\right)\frac{Da}{2}k\|u\|_\Gamma ds + \int_0^t e^{\frac{Da}{2}s}\|v(s=0)\|_\Gamma ds \\
\|v\|_\Gamma &\leq \int_0^t k\left(e^{\frac{Da}{2}s} - 1\right)\|u\|_\Gamma ds
\end{aligned} \tag{4.15}$$

where we used Gronwall's inequality.
Now substitute $\phi = u$ to get

$$\begin{aligned}
\frac{d}{dt}\|u\|_\Omega^2 + \|\nabla u\|_\Omega^2 + \|u\|_\Gamma^2 &\leq \|u\|_\Gamma\|v\|_\Gamma \\
&\leq \frac{1}{2}\|u\|_\Gamma^2 + \frac{1}{2}\|v\|_\Gamma^2
\end{aligned}$$

where this step is justified by the Cauchy-Schwarz inequality.

Since the terms $\|\nabla u\|_\Omega^2$ and $\|u\|_\Gamma^2$ are both positive, integration gives us

$$\begin{aligned}
\|u\|_\Omega^2 &\leq \frac{1}{2}\int_0^t \|u\|_\Gamma^2 ds + \frac{1}{2}\int_0^t \|v\|_\Gamma^2 ds \\
&\leq \frac{1}{2}\int_0^t \|u\|_\Gamma^2 ds + \frac{1}{2}\int_0^t k^2 \left(e^{\frac{Da}{2}s} - 1\right)^2 \|u\|_\Gamma^2 ds \\
&\leq \frac{1}{2}\int_0^t \left(k^2 \left(e^{\frac{Da}{2}s} - 1\right)^2 + 1\right) \|u\|_\Omega^2 ds
\end{aligned}$$

Now apply Gronwall's inequality once again to directly get

$$\|u\|_\Omega \leq 0$$

and conclude that $u = 0$ a.e. in Ω and since (4.15) must hold also $v = 0$ a.e. in Γ.

Remark 4.6.1. *Recall that the existence was obtained as a limit of a sequence $\tau \searrow 0$ of the pair (U_τ, V_τ). Since the solution is unique, it follows that for any sequence $\tau \searrow 0$ the sequence (U_τ, V_τ) converges to (u, v).*

5 Unfolding techniques and homogenization

In this chapter we will first discuss how the model given in Section 3.1 is translated into a geometry containing an oscillatory boundary. For this purpose we need to properly describe the geometry.
Furthermore, in Section 5.3 we will give a description of the periodic unfolding method, used to study the homogenization of multi-scale periodic problems. In particular, we look at the so called unfolding operator. This operator was introduced by Cioranescu et al. in [2], but a similar concept can also be found in [13] and [1]. Here we consider a version for oscillating boundary cases introduced in [3]. The unfolding operator is used to convert integrals over ε-depending domains to integrals over a fixed domain. This means it can be used for both the domain and the boundary.

5.1 Geometry

Let $h : \mathbb{R} \mapsto [-1, 0]$ be a given smooth 1-periodic function and let $\Omega^\varepsilon \subset \mathbb{R}^2$ be the following open bounded set:

$$\Omega^\varepsilon := \left\{ (x, y) \in \mathbb{R}^2 \middle| x \in (0, 1), y \in \left(h^\varepsilon(x), 1\right) \right\},$$

where

$$h^\varepsilon(x) = \varepsilon h\left(\frac{x}{\varepsilon}\right).$$

Having $\partial\Omega^\varepsilon$ as the boundary of Ω^ε, the oscillatory boundary $\Gamma^\varepsilon \subset \partial\Omega^\varepsilon$ is defined as

$$\Gamma^\varepsilon := \left\{ (x, y) \in \mathbb{R}^2 \middle| x \in (0, 1), y = \varepsilon h\left(\frac{x}{\varepsilon}\right) \right\}.$$

Since Γ^ε is periodic, we scale one period and define Γ

$$\Gamma := \{(x, y) : x \in (0, 1), y = h(z)\}.$$

Figure 5.2 is a sketch of this geometry.

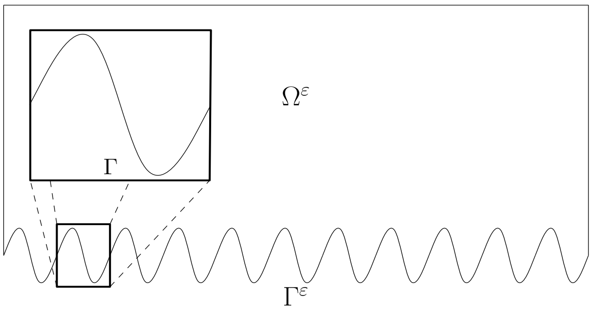

Figure 5.1: Ω^ε is the considered domain. The boundary Γ^ε is defined by a periodic function, of which we will call one period Γ. This domain stays fixed in time, for a given ε.

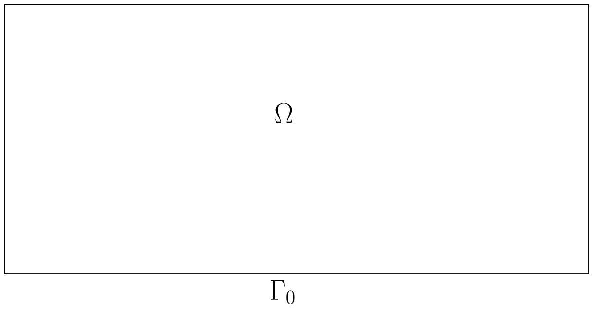

Figure 5.2: Ω is the homogenized domain. The boundary Γ_0 is a flat line.

Let $\Omega := (0,1) \times (0,1)$ be the simplified domain that we will refer to as the homogenized domain. Please note that this implies that $\Omega \subset \Omega^\varepsilon$ as $h^\varepsilon \leq 0$. The boundary of this domain is defined in the following way:

$$\Gamma_0 := \left\{ (x,y) \in \mathbb{R}^2 \middle| x \in (0,1),\, y = 0 \right\},$$

For the remainder of this thesis, we define:

$$\begin{aligned} \Omega^T &:= \Omega \times (0,T), \\ \Gamma_0^T &:= \Gamma_0 \times (0,T), \\ \Omega^{\varepsilon T} &:= \Omega^\varepsilon \times (0,T), \\ \Gamma^{\varepsilon T} &:= \Gamma^\varepsilon \times (0,T). \end{aligned}$$

5.2 Weak form of the adsorption and desorption model

In Chapter 3 we have derived the following equations for the adsorption and desorption model, that we can use on the given geometry:

Problem 5.2.1. *Find u, v such that*

$$\left\{ \begin{array}{rcll} \partial_t u - \Delta u &=& 0 & \text{in } \Omega^\varepsilon \times (0,T), \\ -\partial_\nu u &=& \partial_t v & \text{on } \Gamma^\varepsilon \times (0,T), \\ \partial_t v &=& Da\,(ku - v) & \text{on } \Gamma^\varepsilon \times (0,T), \\ u &=& 0 & \text{on } \partial\Omega^\varepsilon / \Gamma^\varepsilon \times (0,T), \\ u &=& u_I & \text{in } \Omega^\varepsilon \text{ for } t = 0, \\ v &=& v_I & \text{on } \Gamma^\varepsilon \text{ for } t = 0. \end{array} \right. \tag{5.1}$$

As in Chapter 4 we consider weak solutions to Problem 5.2.1. For the sake of clarity we will repeat the definition here:

Definition 5.2.1 (Weak form of the adsorption and desoprtion model)**.** *A weak solution of Problem 5.2.1 is a pair* $(u^\varepsilon, v^\varepsilon)$ *such that*

$$\begin{aligned} u^\varepsilon \in & L^2\left((0,T)\,;H^1\left(\Omega^\varepsilon\right)\right), \\ \partial_t u^\varepsilon \in & L^2\left((0,T)\,;H^{-1}\left(\Omega^\varepsilon\right)\right), \\ v^\varepsilon \in & H^1\left((0,T)\,;L^2\left(\Gamma^\varepsilon\right)\right), \end{aligned}$$

and for any $\phi \in L^2\left(0,T;H^1_{0,\Gamma}\left(\Omega^\varepsilon\right)\right), \theta \in L^2\left(0,T;L^2\left(\Gamma^\varepsilon\right)\right)$

$$\begin{aligned} \int\limits_{\Omega^\varepsilon} \partial_t u^\varepsilon \phi dx + \int\limits_{\Omega^\varepsilon} \nabla u^\varepsilon \nabla \phi dx &= -\int\limits_{\Gamma^\varepsilon} \partial_t v^\varepsilon \phi ds, \\ \int\limits_{\Gamma^\varepsilon} \partial_t v^\varepsilon \theta ds &= \int\limits_{\Gamma^\varepsilon} \left(Da\left(ku^\varepsilon - v^\varepsilon\right)\right)\theta ds. \end{aligned}$$

5.3 Boundary unfolding operator

As we take the limit $\varepsilon \to 0$ the domain Ω^ε changes into Ω. However, for the oscillatory boundary Γ^ε, taking the limit $\varepsilon \to 0$ is not so straightforward. We will for this purpose define an unfolding operator.

In this section we will use both the integer and the fractional part of a real number. We will use the notation $\lfloor . \rfloor : \mathbb{R} \to \mathbb{Z}$ for the integer part (one can see this as the floor function) and $\{.\}$ as the fractional part. Shortly said, $x = \lfloor x \rfloor + \{x\}\, \forall x \in \mathbb{R}$.

Definition 5.3.1. *Let* $\phi^\varepsilon : (0,1)\times\Gamma \to \Gamma^\varepsilon$ *be defined as* $(x,(z,h(z))) \mapsto \left(\varepsilon \left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon z, \varepsilon h(z)\right)$. *The unfolding operator* T^ε *maps a function* $u : \Gamma^\varepsilon \to \mathbb{R}$ *to the function* $u \circ \phi^\varepsilon : (0,1)\times\Gamma \to \mathbb{R}$.

T^ε has some properties that will be used, therefore the following propositions are stated:

Proposition 5.3.1. T^ε *is linear.*

Proposition 5.3.2. *Let* u,v *be functions* $\Gamma^\varepsilon \to \mathbb{R}$. *Then* $T^\varepsilon(uv) = T^\varepsilon u T^\varepsilon v$.

The proofs for Proposition 5.3.1 and Proposition 5.3.2 are straightforward and therefore omitted.

Proposition 5.3.3. *Let $u \in L^1(\Gamma^\varepsilon)$ and $N := \frac{1}{\varepsilon}$. Then*

$$\int\limits_{(0,1)\times\Gamma} T^\varepsilon u\left(x,(z,h(z))\right) dsdx = \int\limits_{\Gamma^\varepsilon} u\left(y, \varepsilon h\left(\frac{y}{\varepsilon}\right)\right) d\tilde{s}$$

Proof. Let $u \in L^1(\Gamma^\varepsilon)$ and let $N := \frac{1}{\varepsilon}$. Then

$$\begin{aligned}
\int\limits_{(0,1)\times\Gamma} T^\varepsilon u\left(x,(z,h(z))\right) dsdx &= \int\limits_{(0,1)\times\Gamma} u\left(\varepsilon\left(\left\lfloor\frac{x}{\varepsilon}\right\rfloor + z\right), \varepsilon h(z)\right) dsdx \\
&= \int_0^1\int_0^1 u\left(\varepsilon\left(\left\lfloor\frac{x}{\varepsilon}\right\rfloor + z\right), \varepsilon h(z)\right)\sqrt{1+(\varepsilon h'(z))^2}dzdx \\
&= \sum_{k=0}^{N-1}\int_{k\varepsilon}^{(k+1)\varepsilon}\int_0^1 u\left(\varepsilon\left(\left\lfloor\frac{x}{\varepsilon}\right\rfloor + z\right), \varepsilon h(z)\right)\sqrt{1+(\varepsilon h'(z))^2}dzdx \\
&= \sum_{k=0}^{N-1}\int_{k\varepsilon}^{(k+1)\varepsilon}\int_0^1 u\left(\varepsilon k + \varepsilon z, \varepsilon h(z)\right)\sqrt{1+(\varepsilon h'(z))^2}dzdx \\
&= \sum_{k=0}^{N-1}\varepsilon\int_0^1 u\left(\varepsilon k + \varepsilon z, \varepsilon h(z)\right)\sqrt{1+(\varepsilon h'(z))^2}dz
\end{aligned}$$

Using respectively $y := \varepsilon k + \varepsilon z$ and the periodicity of h, we get:

$$\begin{aligned}
&\sum_{k=0}^{N-1}\varepsilon\int_0^1 u\left(\varepsilon k + \varepsilon z, \varepsilon h(z)\right)\sqrt{1+(\varepsilon h'(z))^2}dz \\
&\quad= \sum_{k=0}^{N-1}\varepsilon\int_{k\varepsilon}^{(k+1)\varepsilon} u\left(y, \varepsilon h\left(\frac{y}{\varepsilon}-k\right)\right)\sqrt{1+\left(\varepsilon h'\left(\frac{y}{\varepsilon}-k\right)\right)^2}d\left(\frac{y}{\varepsilon}-k\right) \\
&\quad= \sum_{k=0}^{N-1}\int_{k\varepsilon}^{(k+1)\varepsilon} u\left(y, \varepsilon h\left(\frac{y}{\varepsilon}\right)\right)\sqrt{1+\left(\varepsilon h'\left(\frac{y}{\varepsilon}\right)\right)^2}dy \\
&\quad= \int_0^1 u\left(y, \varepsilon h\left(\frac{y}{\varepsilon}\right)\right)\sqrt{1+\left(\varepsilon h'\left(\frac{y}{\varepsilon}\right)\right)^2}dy \\
&\quad= \int\limits_{\Gamma^\varepsilon} u\left(y, \varepsilon h\left(\frac{y}{\varepsilon}\right)\right)d\tilde{s}
\end{aligned}$$

□

Proposition 5.3.4. *Let* $u \in L^2(\Gamma^\varepsilon)$. *Then* $T^\varepsilon u \in L^2((0,1)\times\Gamma)$ *and* T^ε *is a linear isometry beween* $L^2(\Gamma^\varepsilon)$ *and* $L^2((0,1)\times\Gamma)$.

Proof. Suppose that $u \in L^2(\Gamma^\varepsilon)$. Then $|u|^2 \in L^1(\Gamma^\varepsilon)$. Using Propositions 5.3.2 and 5.3.3 we find

$$\int\limits_{(0,1)\times\Gamma} \left|T^\varepsilon u\right|^2 dx = \int\limits_{(0,1)\times\Gamma} T^\varepsilon |u|^2 dx = \int\limits_{\Gamma^\varepsilon} |u|^2 dx < \infty$$

This calculations also show that $\|T^\varepsilon u\|_{L^2((0,1)\times\Gamma)} = \|u\|_{L^2(\Gamma^\varepsilon)}$. Together with Proposition 5.3.1 this implies that T^ε is a linear isometry beween $L^2(\Gamma^\varepsilon)$ and $L^2((0,1)\times\Gamma)$. □

5.4 Homogenization

We will use the properties and results of both Chapter 2 and Chapter 4 to give estimates that, given the problem described at Section 3.1, will help us to homogenize both domain and boundary.
We will use the manner in which we construct the homogenized domain from the oscillatory domain to our advantage, as estimates carry over immediately. We however do need to show that as $\varepsilon \to 0$, the sequence u^ε converges to a limit independent of ε.
For the boundary, we will use the periodic unfolding operator as defined in Section 5.3, and show some convergence results with respect to this operator. More specific, we will homogenize the variational problem given in Definition 5.2.1 by considering a sequence u^ε of solutions, with an identified limit in a fixed domain.
The limits acquired from the domain and the boundary homogenization for u^ε should not contradict each other i.e. their difference should be small enough.

5.4.1 Homogenization in the domain

Because of the chosen construction of domain Ω^ε it is possible to split Ω^ε into $\Omega^\varepsilon\backslash\Omega$ and Ω. This results in the following equalities:

$$\int\limits_{\Omega^\varepsilon} \nabla u^\varepsilon \nabla\phi dx = \int\limits_{\Omega^\varepsilon\backslash\Omega} \nabla u^\varepsilon \nabla\phi dx + \int\limits_{\Omega} \nabla u^\varepsilon \nabla\phi dx$$

$$\int\limits_{\Omega^\varepsilon} \partial_t u^\varepsilon \phi dx = \int\limits_{\Omega^\varepsilon\backslash\Omega} \partial_t u^\varepsilon \phi dx + \int\limits_{\Omega} \partial_t u^\varepsilon \phi dx$$

Now we would like that both integrals over $\Omega^\varepsilon\backslash\Omega$ tend to zero as $\varepsilon \to 0$. For that reason, we propose the following direct consequence of the Dominated convergence theorem (see Theorem 2.6.1):

Proposition 5.4.1. *For any function* $f \in L^1(\Omega)$*, with* $E \subset \Omega$*, it holds that* $\int_E |f| \to 0$ *as* $\mu(E)$ *(the measure of* E*)* $\to 0$*.*

Lemma 5.4.1. *As* $\varepsilon \to 0$*, for any* $\phi \in H^1\left(0, T; L^2\left(\Omega^\varepsilon\right)\right)$

$$\int_0^T \int_{\Omega^\varepsilon \setminus \Omega} \partial_t u^\varepsilon \phi dx dt \to 0.$$

Proof. Suppose $\varepsilon \to 0$. Since

$$\begin{aligned}
\int_0^T \int_{\Omega^\varepsilon \setminus \Omega} -u^\varepsilon \partial_t \phi dx dt &\leq \|u^\varepsilon\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \|\partial_t \phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \\
&\leq \|u^\varepsilon\|_{L^2\left(0,T;L^2(\Omega^\varepsilon)\right)} \|\partial_t \phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \\
&\leq C \|\partial_t \phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)}
\end{aligned}$$

and since we know $\partial_t \phi \in L^2\left(0, T; L^2\left(\Omega^\varepsilon\right)\right)$, we have $|\partial_t \phi|^2 \in L^2\left(0, T; L^1\left(\Omega^\varepsilon\right)\right)$, and because of Proposition 5.4.1 we can conclude that

$$\int_0^T \int_{\Omega^\varepsilon \setminus \Omega} \partial_t u^\varepsilon \phi dx dt \to 0.$$

□

Lemma 5.4.2. *As* $\varepsilon \to 0$*, for any* $\phi \in L^2\left(0, T; H^1\left(\Omega^\varepsilon\right)\right)$

$$\int_0^T \int_{\Omega^\varepsilon \setminus \Omega} \nabla u^\varepsilon \nabla \phi dx dt \to 0.$$

Proof. Suppose $\varepsilon \to 0$. Since

$$\begin{aligned}
\int_0^T \int_{\Omega^\varepsilon \setminus \Omega} \nabla u^\varepsilon \nabla \phi dx dt &\leq \|\nabla u^\varepsilon\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \|\nabla \phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \\
&\leq \|\nabla u^\varepsilon\|_{L^2\left(0,T;L^2(\Omega^\varepsilon)\right)} \|\phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)} \\
&\leq C \|\phi\|_{L^2\left(0,T;L^2(\Omega^\varepsilon \setminus \Omega)\right)}
\end{aligned}$$

and since $\phi \in L^2\left(0,T;L^2\left(\Omega^\varepsilon\right)\right)$, we have $|\phi|^2 \in L^2\left(0,T;L^1\left(\Omega^\varepsilon\right)\right)$. Using Proposition 5.4.1 we can conclude that

$$\int_0^T \int_{\Omega^\varepsilon\setminus\Omega} \nabla u^\varepsilon \nabla\phi dx dt \to 0. \qquad \square$$

The estimates we found in Chapter 4 carry over for the restriction of u^ε to Ω (which we will still call u^ε because it makes writing more simplified) because we chose $\Omega \subset \Omega^\varepsilon$. Using those estimates, we have:

Lemma 5.4.3. *Along a sequence $\varepsilon \searrow 0$,*

$$\nabla u^\varepsilon \rightharpoonup \nabla\tilde{u_0} \quad \textit{weakly in} \quad L^2\left(0,T;L^2(\Omega)\right). \tag{5.2}$$

$$u^\varepsilon \to \tilde{u_0} \quad \textit{strongly in} \quad L^2\left(0,T;L^2(\partial\Omega)\right). \tag{5.3}$$

Proof. The convergence in (5.2) is a direct consequence of (4.13).
To become able to prove (5.3), we note that $\partial_t u^\varepsilon \in L^2\left(0,T;H^*(\Omega)\right)$ where H^* is the dual of $H_0^1(\Omega)$, referring to the space of H^1 functions that have homogenous Dirichlet boundary conditions on $\partial\Omega$. Note the subtle difference between the earlier defined $H^1_{0,\Gamma}(\Omega)$ where the homogenous Dirichlet boundary conditions were only taken on $\partial\Omega/\Gamma_0$.
With $u^\varepsilon \in L^2\left(0,T;H^1_{0,\Gamma}(\Omega)\right)$ and $\partial_t u^\varepsilon \in L^2\left(0,T;H^*(\Omega)\right)$, we can conclude that u^ε converges strongly in $L^2\left(0,T;L^2(\Omega)\right)$.
Following the proof of the trace theorem (see [7], Chapter 5.5), we have that

$$\begin{aligned}
&\|u^\varepsilon - \tilde{u_0}\|_{L^2(0,T;L^2(\partial\Omega))} \\
&\qquad \le C\|u^\varepsilon - \tilde{u_0}\|_{L^2(0,T;L^2(\Omega))}\left(\|u^\varepsilon - \tilde{u_0}\|_{L^2(0,T;L^2(\Omega))} + \|\nabla\left(u^\varepsilon - \tilde{u_0}\right)\|_{L^2(0,T;L^2(\Omega))}\right) \\
&\qquad \le C\|u^\varepsilon - \tilde{u_0}\|_{L^2(0,T;L^2(\Omega))}
\end{aligned}$$

where we used the semi-continuity of the norms, the bounds on the gradients, and Cauchy Schwarz. Estimate (5.3) follows. $\square$

5.4.2 Homogenization at the boundary

If we define T^ε as the unfolding operator on the boundary Γ^ε (as in Section 5.3) we get that:

$$\int_{\Gamma^\varepsilon} Da\left(\left(ku^\varepsilon - v^\varepsilon\right)\phi\right)ds = Da\ k\int_0^1\int_\Gamma T^\varepsilon u^\varepsilon T^\varepsilon\phi dx d\xi - Da\int_0^1\int_\Gamma T^\varepsilon v^\varepsilon T^\varepsilon\phi dx d\xi$$

for all $\phi \in L^2\left(0,T;L^2\left(\Gamma^\varepsilon\right)\right)$.

Theorem 5.4.1. *For $u^\varepsilon \in H^1(\Omega^\varepsilon)$ uniform bounded with respect to ε, $T^\varepsilon u^\varepsilon \to u_0$ strongly in $L^2(\Gamma \times (0,1))$.*

Proof. Since $\|u^\varepsilon\|_{H^1(\Omega^\varepsilon)} \leq C$, the trace theorem tells us that $\|u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma^\varepsilon)} \leq C$ where

$$\|u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma^\varepsilon)} = \int\limits_{\Gamma^\varepsilon}\int\limits_{\Gamma^\varepsilon} \frac{|u^\varepsilon(x, h^\varepsilon(x)) - u^\varepsilon(y, h^\varepsilon(y))|^2}{|x-y|^3} dxdy$$

Since

$$\begin{aligned}
\|T^\varepsilon u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma\times(0,1))} &= \int\limits_{\Gamma\times(0,1)}\int\limits_{\Gamma\times(0,1)} \frac{\left|T^\varepsilon u^\varepsilon(x,\xi) - T^\varepsilon u^\varepsilon\left(y,\xi'\right)\right|^2}{\left|\varepsilon\left(\lfloor\frac{x}{\varepsilon}\rfloor - \lfloor\frac{y}{\varepsilon}\rfloor + \xi - \xi'\right)\right|^3} dxdy \\
&= \sum_k \sum_{k'} \int\limits_{k\varepsilon}^{(k+1)\varepsilon}\int\limits_{k'\varepsilon}^{(k'+1)\varepsilon}\int\limits_0^1\int\limits_0^1 \frac{\left|u^\varepsilon(\varepsilon k + \varepsilon\xi, h^\varepsilon(k+\xi)) - u^\varepsilon\left(\varepsilon k' + \varepsilon\xi', h^\varepsilon(k'+\xi')\right)\right|^2}{\left|\varepsilon\left(k + \xi - k' - \xi'\right)\right|^3} d\xi d\xi' dxdy \\
&= \int\limits_{\Gamma^\varepsilon}\int\limits_{\Gamma^\varepsilon} \frac{|u^\varepsilon(z_1, h^\varepsilon(z_1)) - u^\varepsilon(z_2, h^\varepsilon(z_2))|^2}{|z_1 - z_2|^3} dz_1 dz_2 \\
&= \|u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma^\varepsilon)}
\end{aligned}$$

where $z_1 = \varepsilon k + \varepsilon\xi$ and $z_2 = \varepsilon k' + \varepsilon\xi'$.
Since $\|u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma^\varepsilon)} \leq C$ it follows that $\|T^\varepsilon u^\varepsilon\|_{H^{\frac{1}{2}}(\Gamma\times(0,1))} \leq C$. So $T^\varepsilon u^\varepsilon \rightharpoonup u_0$ weakly in $H^{\frac{1}{2}}(\Gamma \times (0,1))$. So $T^\varepsilon u^\varepsilon \to u_0$ strongly in $L^2(\Gamma \times (0,1))$. □

5.4.3 Connecting the limits

It remains to be shown that the trace of the limits found in Sections 5.4.1 and 5.4.2 coincide. We prove this by the following theorem:

Theorem 5.4.2. *Let u_0 be the limit found in Theorem 5.4.1 and $\tilde{u_0}$ be the limit found in Lemma 5.4.3. Then for almost every t,*

$$\|u_0(t,x,(z,h(z))) - \tilde{u_0}(t,x,y=0)\|_{L^1\left(0,T;L^1((0,1)\times\Gamma)\right)} = 0.$$

Proof. Let

$$I := \int\limits_0^T\int\limits_0^1\int\limits_\Gamma \|u_0(t,x,z) - \tilde{u_0}(t,x,y=0)\| dsdxdt.$$

By the triangle inequality we find

$$\begin{aligned}
I \leq & \int_0^T \int_0^1 \int_\Gamma \left\| u_0\left(t, x, (z, h(z))\right) - T^\varepsilon u^\varepsilon\left(t, x, (z, h(z))\right) \right\| dsdxdt \\
+ & \int_0^T \int_0^1 \int_\Gamma \left\| u^\varepsilon\left(t, \varepsilon\left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon z, \varepsilon h(z)\right) - u^\varepsilon\left(t, \varepsilon\left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon z, 0\right) \right\| dsdxdt \\
+ & \int_0^T \int_0^1 \int_\Gamma \left\| u^\varepsilon\left(t, \varepsilon\left\lfloor \frac{x}{\varepsilon} \right\rfloor + \varepsilon z, 0\right) - u^\varepsilon\left(t, x, 0\right) \right\| dsdxdt \\
+ & \int_0^T \int_0^1 \int_\Gamma \left\| u^\varepsilon\left(t, x, y = 0\right) - \tilde{u_0}\left(t, x, y = 0\right) \right\| dsdxdt
\end{aligned}$$

Now we will show each of these four terms tend to zero. For the first term we have

$$\left\| u_0\left(t, x, (z, h(z))\right) - T^\varepsilon u^\varepsilon\left(t, x, (z, h(z))\right) \right\|_{L^1((0,T)\times(0,1)\times\Gamma)} \to 0$$

since $T^\varepsilon u^\varepsilon \to u_0$ in $L^2\left((0, T) \times (0, 1) \times \Gamma\right)$.
For the second term, we use the Cauchy-Schwarz inequality to get

$$\begin{aligned}
\int_0^T \int_0^1 \int_\Gamma \left\| \int_0^{\varepsilon h(z)} \partial_\xi u^\varepsilon \right\| & \leq \int_0^T \int_0^1 \int_\Gamma \left(\varepsilon \left\| h \right\|^{\frac{1}{2}} \int_0^{\varepsilon h} \left\| \partial_z u^\varepsilon \right|^2 \right)^{\frac{1}{2}} \\
& \leq C\varepsilon^{\frac{1}{2}} \left| \partial_z u^\varepsilon \right|_{L^2(0,T;L^2(\Omega^\varepsilon))} \leq C\sqrt{\varepsilon} \left| \nabla u^\varepsilon \right|_{L^2(0,T;L^2(\Omega^\varepsilon))}
\end{aligned}$$

which is bounded by $C\sqrt{\varepsilon}$ since $u^\varepsilon \in L^2\left(0, T; H^1(\Omega^\varepsilon)\right)$. This implies that this term goes to zero as $\varepsilon \searrow 0$.
The third term represents the translation of u^ε by εz in the x direction. Using $\|z\| \leq 1$ and Lemma 4.12 of [10], this term approaches 0 as $\varepsilon \searrow 0$.
For the last term we find

$$\begin{aligned}
& \left| u^\varepsilon\left(t, x, y = 0\right) - \tilde{u_0}\left(t, x, y = 0\right) \right|_{L^1((0,T)\times(0,1)\times\Gamma)} \\
& \qquad = \left\| \Gamma \right\| \left| u^\varepsilon\left(t, x, y = 0\right) - \tilde{u_0}\left(t, x, y = 0\right) \right|_{L^1((0,T)\times(0,1))}
\end{aligned}$$

which converges to 0 because of the result of Lemma 5.4.3. □

5.4.4 Upscaled model

Now we have established that the trace of $\tilde{u_0}$ is equal to u_0, we can denote both limits by u for our convenience.

Choose $\phi \in H^1((0,T)\times\Omega)$ s.t. $\phi(T,x)=0$ and $\theta \in L^2\left(0,T;L^2((0,1)\times\Gamma)\right)$ to get the upscaled equations

$$
\begin{aligned}
-\int_0^T\int_\Omega u\,(\partial_t\phi)\,dxdt+\int_0^T\int_\Omega \nabla u\nabla\phi dxdt \quad &+ \quad \int_0^T\int_{(0,1)\times\Gamma}(\partial_t v)\,\phi ds=\int_\Omega u_I\phi(x,0)dx\\
\int_0^T\int_{(0,1)\times\Gamma}(\partial_t v)\,\theta dxdsdt \quad &= \quad \int_0^T\int_{(0,1)\times\Gamma}\left(Da\left(ku^\varepsilon-v^\varepsilon\right)\right)\theta dxdsdt.
\end{aligned}
$$

6 Numerical simulations

To validate our approximation of the upscaled problem to the original problem, we now turn to numerical simulations. For these simulations, we use COMSOL Multiphysics. We will shortly discuss choices that have been made in geometry, boundary and initial values, and methods used. The gathered data are analyzed using MATLAB. We will show some results of this process and also state some relevant conclusions.
Looking at the geometry as introduced in Section 5.1, we wish to keep the desired property $\Omega \subset \Omega^{\varepsilon}$. To guarantee this, we define

$$\Gamma^{\varepsilon} := \left\{(x, y) : x \in (0, 1), y = \varepsilon \left(-1.1 + \sin\left(\frac{\pi}{2} + 2\pi \frac{x}{\varepsilon}\right)\right)\right\}.$$

We perform simulations for various values of ε and try to determine how the outcome relates to the upscaled geometry.
We use the finite element method with BDF time stepping as implemented in COMSOL Multiphysics to solve the equations. Time steps will have size 0.1, varying from 0 to 1. The initial conditions are chosen as follows:

$$\begin{aligned} u^{\varepsilon}(x, y, t = 0) &= 1 \qquad \text{in } \Omega^{\varepsilon}, \\ v^{\varepsilon}(x, t = 0) &= 0.2 \qquad \text{on } \Gamma^{\varepsilon}, \\ u(x, y, t = 0) &= 1 \qquad \text{in } \Omega, \\ v(x, t = 0) &= 0.2 \qquad \text{on } \Gamma_0. \end{aligned}$$

To prevent any discontinuities at the boundary, the following boundary conditions are chosen:

$$\begin{aligned} u^{\varepsilon}(x, y, t) &= 1 \qquad \text{at } \left(\partial\Omega^{\varepsilon} / \Gamma^{\varepsilon}\right), \\ u(x, y, t) &= 1 \qquad \text{at } \left(\partial\Omega / \Gamma_0\right), \end{aligned}$$

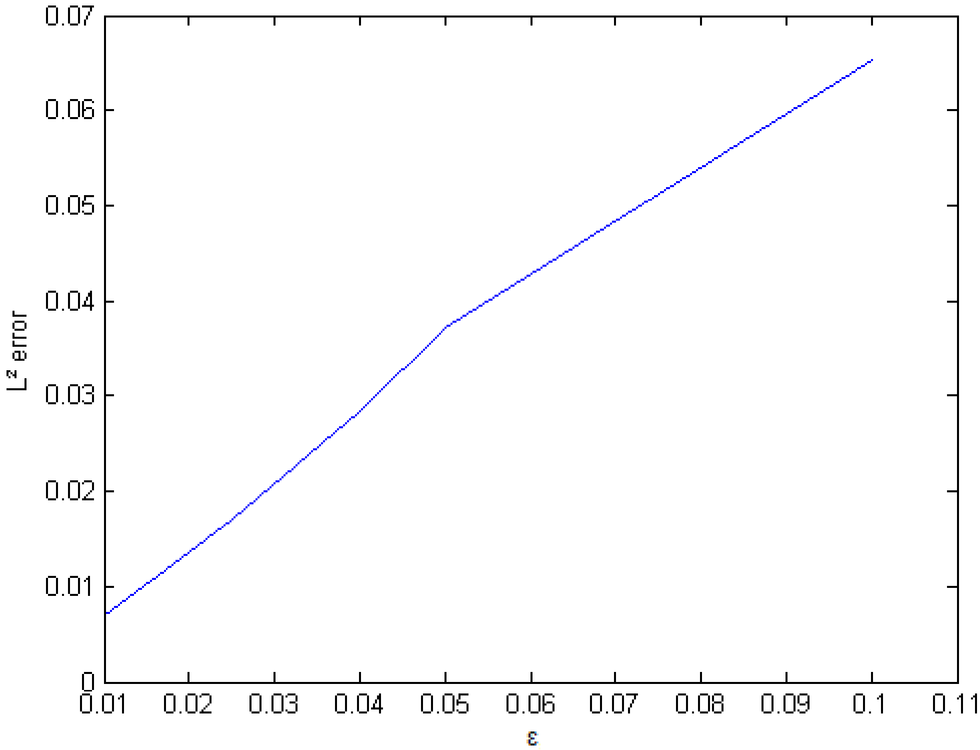

Figure 6.1: The error $E_{\varepsilon}^{u_{dom}}$ for various values of ε, where $Da = 1, k = 1$.

6.1 $Da = 1, k = 1$

6.1.1 Error in the domain

We can consider the $L^2(\Omega \times 0, T)$ error when computing the data for various ε on a regular rectangular grid of size 201 by 201 for both x and $y \in (0, 1)$ and comparing that data to the data found in the upscaled model. We assume that the error will be of order ε^{α} for some $\alpha \in \mathbb{R}$,

$$E_{\varepsilon}^{u_{dom}} := \left\| u^{\varepsilon} - u \right\|_{L^2(\Omega \times 0, T)} \leq C\varepsilon^{\alpha}.$$

When plotting the L^2-errors with respect to the value of ε, this results in Figure 6.1. To give an estimate for α, we determine the ratio

$$\alpha_i = \frac{\log\left(E_{\varepsilon_i}^{u_{dom}}\right) - \log\left(E_{\varepsilon_{i-1}}^{u_{dom}}\right)}{\log\left(\varepsilon_i\right) - \log\left(\varepsilon_{i-1}\right)}, i = 2, ..., 6$$

for various values of ε. The results are given in Table 6.1. We can conclude that the convergence order is close to 1.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{dom}}$	0.0653	0.0372	0.0285	0.0171	0.0135	0.0070
α_i	-	0.8115	1.1995	1.0796	1.0522	0.9540

Table 6.1: Table for L^2 error for concentrations u^ε in the entire domain, where $Da = 1, k = 1$.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{bdry}}$	0.0489	0.0287	0.0210	0.0133	0.0104	0.0052
β_i	-	0.7687	1.3932	0.9741	1.1014	1.0042

Table 6.2: Table for L^2 error for the concentration u on the boundary, where $Da = 1, k = 1$.

6.1.2 Concentration profiles

We compute the full solution for various ε and plot both u and u^ε at respectively Γ and Γ^ε at $t = 0.5$. This plot is shown in Figure 6.2. The largest error are expected to take place at the boundary, due to the oscillations in the boundary. Because of the oscillating boundary, the concentrations u^ε have an oscillating profile whereas the upscaled concentration u is free of oscillations. When ε decreases, u^ε converges to u.
We can do something similar for v and v^ε. The plot of their solutions is shown at Figure 6.3. Both v and v^ε are only defined on the boundary. We see an oscillating profile for v^ε and a non-oscillating v, which meets our expectations. Also, when ε decreases v^ε converges to v.

6.1.3 Order of the error at the boundary

To compute the error of u^ε at the boundary, we calculate

$$E_\varepsilon^{u_{bdry}} := \left\| u^\varepsilon - u \right\|_{L^2(\tilde{\Gamma})} \leq C\varepsilon^\beta$$

at $t = 0.5$ for various values of ε, where $\tilde{\Gamma} := \{(x,0)|x \in (0,1)\}$, To estimate β we compute the ratio

$$\beta_i = \frac{\log\left(E_{\varepsilon_i}^{u_{bdry}}\right) - \log\left(E_{\varepsilon_{i-1}}^{u_{bdry}}\right)}{\log(\varepsilon_i) - \log(\varepsilon_{i-1})}, i = 2, ..., 6$$

and the results can be found in Table 6.2. We can conclude that the convergence order is close to 1. Obviously we can not do the same to compute the error of v^ε, since in

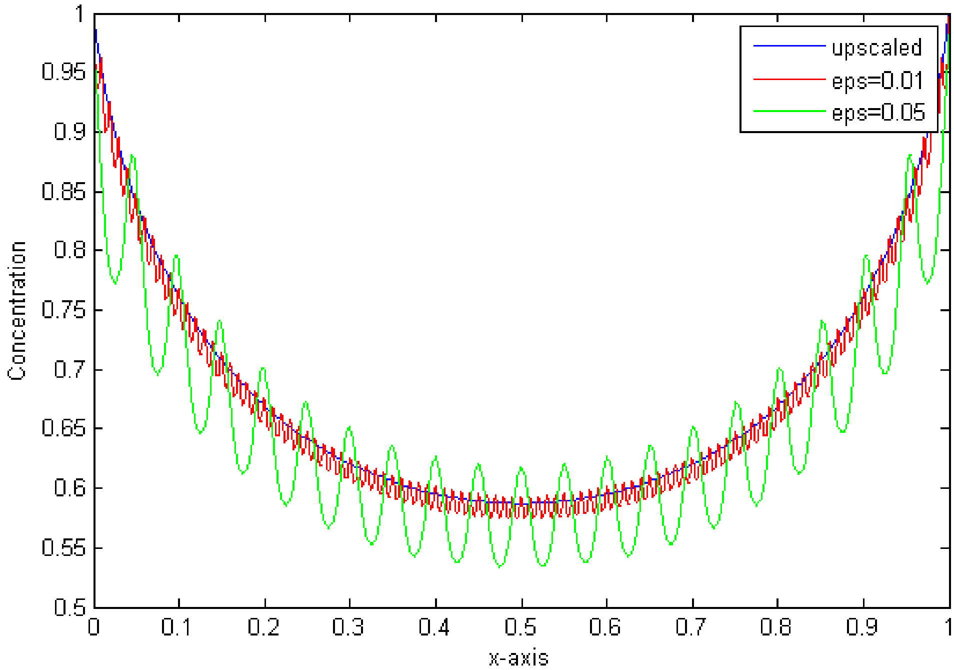

Figure 6.2: Concentrations of u^{ε} ($\varepsilon = 0.01$ and $\varepsilon = 0.05$), and of u on the boundary, where $Da = 1, k = 1$.

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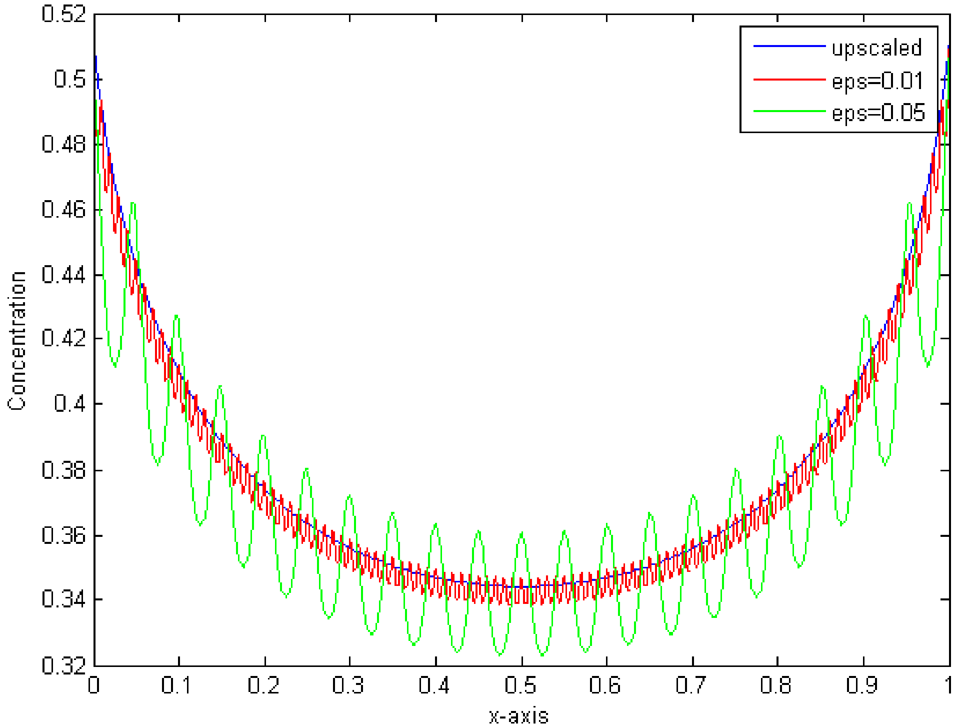

Figure 6.3: Concentrations of v^ε for $\varepsilon = 0.01$ and $\varepsilon = 0.05$, and of v on the boundary, where $Da = 1, k = 1$.

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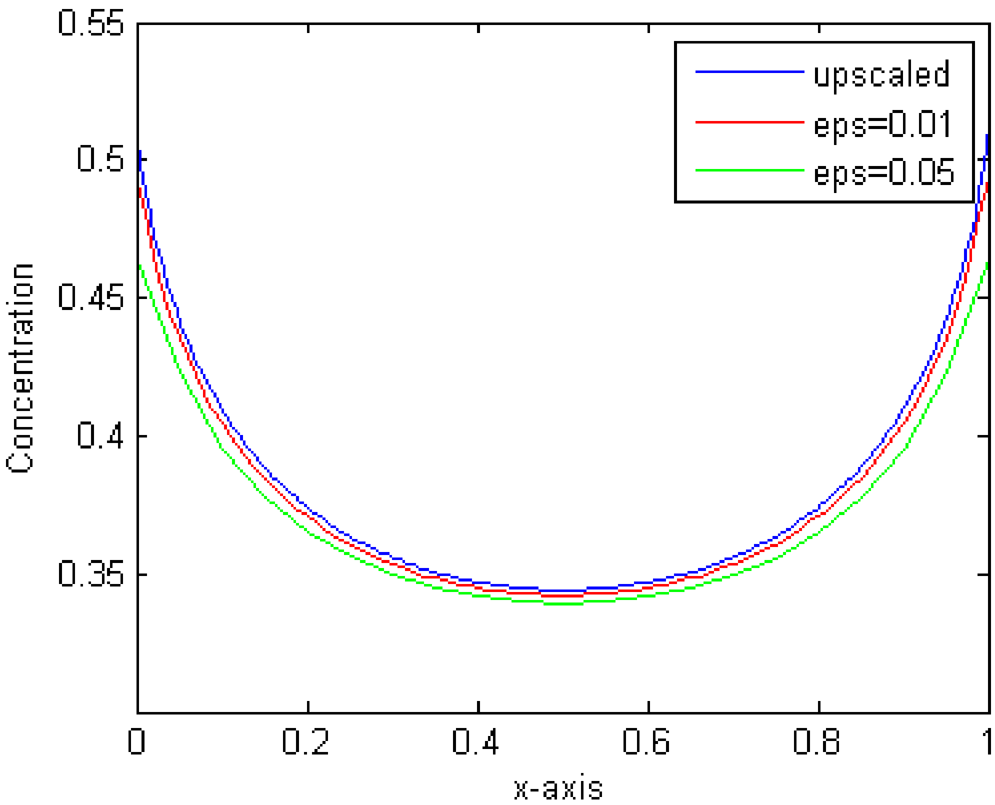

Figure 6.4: Concentrations of $\bar{v^\varepsilon}$ for $\varepsilon = 0.01$ and $\varepsilon = 0.05$, compared to v of the upscaled model.

.

general it is not defined on $\tilde{\Gamma}$. Hence we look at

$$\bar{v^\varepsilon}(x) = \frac{1}{\varepsilon} \int_{\varepsilon\lfloor\frac{x}{\varepsilon}\rfloor-\frac{\varepsilon}{2}}^{\varepsilon\lfloor\frac{x}{\varepsilon}\rfloor+\frac{\varepsilon}{2}} v^\varepsilon ds,$$

the average of v^ε over one period. This we compared with v from the upscaled model, resulting in Figure 6.4. We see that $\bar{v^\varepsilon}$, especially for low values of ε, are a reasonable approximation of v. Now we try to compute

$$E_\varepsilon^{v_{bdry}} := \left\| \bar{v^\varepsilon} - v \right\|_{L^2(0,1))} \leq C\varepsilon^\gamma$$

for various values of ε. To estimate γ we compute the ratio

$$\gamma_i = \frac{\log\left(E_{\varepsilon_i}^{v_{bdry}}\right) - \log\left(E_{\varepsilon_{i-1}}^{v_{bdry}}\right)}{\log(\varepsilon_i) - \log(\varepsilon_{i-1})}, i = 2, ..., 6$$

and the results can be found in Table 6.3. The convergence order is again close to 1.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{v_{bdry}}$	0.0370	0.0205	0.0180	0.0111	0.0090	0.0055
γ_i	-	0.8493	0.5969	1.0254	0.9573	0.7028

Table 6.3: Table for L^2 error for the adsorbent v, where $Da = 1, k = 1$.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{dom}}$	0.0340	0.0202	0.0161	0.0105	0.0086	0.0045
α_i	-	0.7491	1.0268	0.8998	0.9349	0.9326

Table 6.4: Table for L^2 error for the solute u in the entire domain, where $Da = 10, k = 1$.

6.2 Different values of Da and k

6.2.1 $k = 1, Da = 10$

Error in the domain

We follow the same procedure as we did in Subsection 6.1.1. The results for both $E_\varepsilon^{u_{dom}}$ and α_i are given in Table 6.4. We can conclude that the convergence order is close to 1.

Concentration profiles

We compute the full solution for various ε and plot both u and u^ε at respectively Γ_0 and Γ^ε at $t = 0.5$. This plot is shown in Figure 6.5. When ε decreases, u^ε converges to u. Due to the concentration profile and the oscillations in the boundary, clearly u is a relative bad approximation around $x = 0$ and $x = 1$.

We can do something similar for v and v^ε. The plot of their solutions is shown at Figure 6.6. Both v and v^ε are only defined on the boundary. When ε decreases v^ε converges to v.

Order of the error at the boundary

We follow the same procedure as we did in Subsection 6.1.3. The results for both $E_\varepsilon^{u_{bdry}}$ and β_i are given in Table 6.5. We can conclude that the convergence order is little under 1.

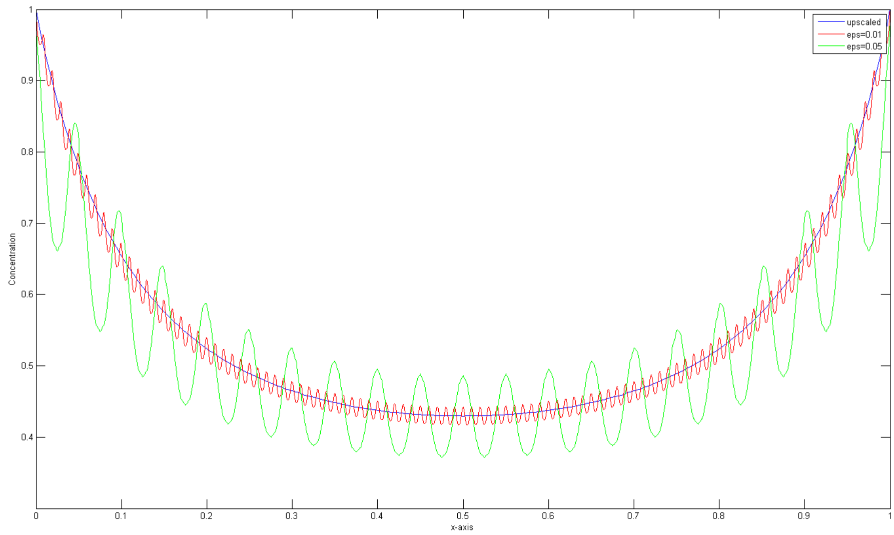

Figure 6.5: Concentrations of u^{ε} ($\varepsilon = 0.01$ and $\varepsilon = 0.05$), and of u on the boundary, where $Da = 10, k = 1$.

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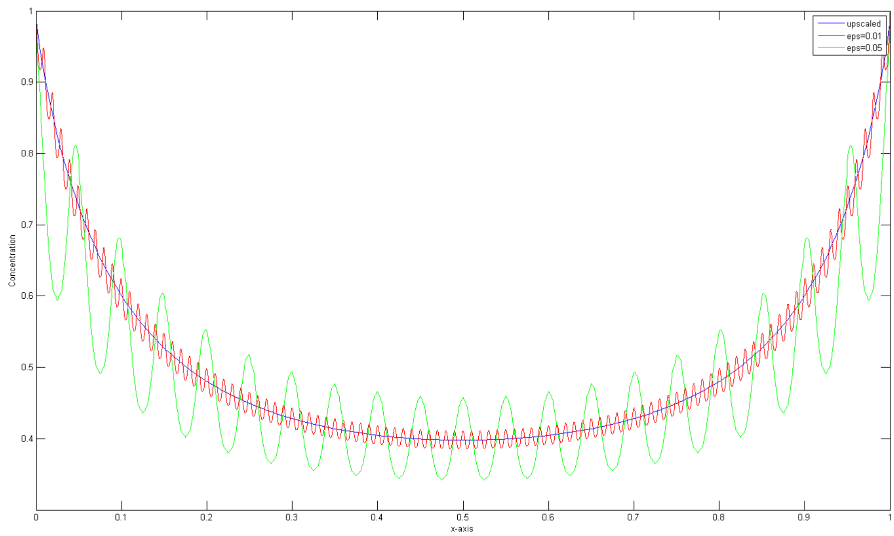

Figure 6.6: Concentrations of v^{ε} ($\varepsilon = 0.01$ and $\varepsilon = 0.05$), and of v on the boundary, where $Da = 10, k = 1$.

.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{bdry}}$	0.0903	0.0545	0.0393	0.0248	0.0196	0.0132
β_i	-	0.7302	1.4622	0.9752	1.0571	0.5771

Table 6.5: Table for L^2 error for the concentrations u on the boundary, where $Da = 10, k = 1$.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{v_{bdry}}$	0.1340	0.0826	0.0733	0.0498	0.0411	0.0210
γ_i	-	0.6975	0.5336	0.8257	0.8605	0.9645

Table 6.6: Table for L^2 error for the adsorbent v, where $Da = 10, k = 1$.

Results for $E_\varepsilon^{v_{bdry}}$ and γ_i can be found in Table 6.6. The convergence order is little under 1.

6.2.2 $k = 10, Da = 1$

Error in the domain

We follow the same procedure as we did in Subsection 6.1.1. The results for both $E_\varepsilon^{u_{dom}}$ and α_i are given in Table 6.7. We can conclude that the convergence order is somewhat below 1.

Concentration profiles

We compute the full solution for various ε and plot both u and u^ε at respectively Γ_0 and Γ^ε at $t = 0.5$. This plot is shown in Figure 6.7. When ε decreases, u^ε converges to u. Due to the concentration profile and the oscillations in the boundary, clearly u is a relative bad approximation around $x = 0$ and $x = 1$.

We can do something similar for v and v^ε. The plot of their solutions is shown at Figure

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{dom}}$	0.0529	0.0343	0.0286	0.0198	0.0164	0.0089
α_i	-	0.6255	0.8103	0.7847	0.8318	0.8833

Table 6.7: Table for L^2 error for the solute u in the entire domain, where $Da = 1, k = 10$.

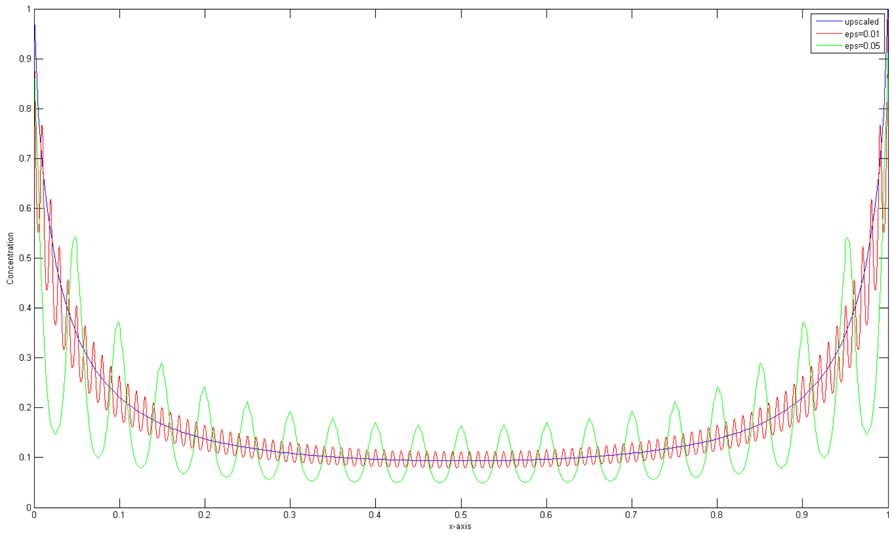

Figure 6.7: Concentrations of u^ε for $\varepsilon = 0.01$ and $\varepsilon = 0.05$, and u on the boundary, where $Da = 1, k = 10$.

.

i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{u_{bdry}}$	0.1657	0.1124	0.0945	0.0673	0.0566	0.0319
β_i	-	0.5602	0.7756	0.7222	0.7782	0.8260

Table 6.8: Table for L^2 error for the concentrations u on the boundary, where $Da = 1, k = 10$.

6.8. Both v and v^ε are only defined on the boundary. When ε decreases v^ε converges to v.

Order of the error at the boundary

We follow the same procedure as we did in Subsection 6.1.3. The results for both $E_\varepsilon^{u_{bdry}}$ and β_i are given in Table 6.8. We can conclude that the convergence order is significantly below 1.

Results for $E_\varepsilon^{v_{bdry}}$ and γ_i can be found in Table 6.9. The convergence order is around $\frac{1}{2}$.

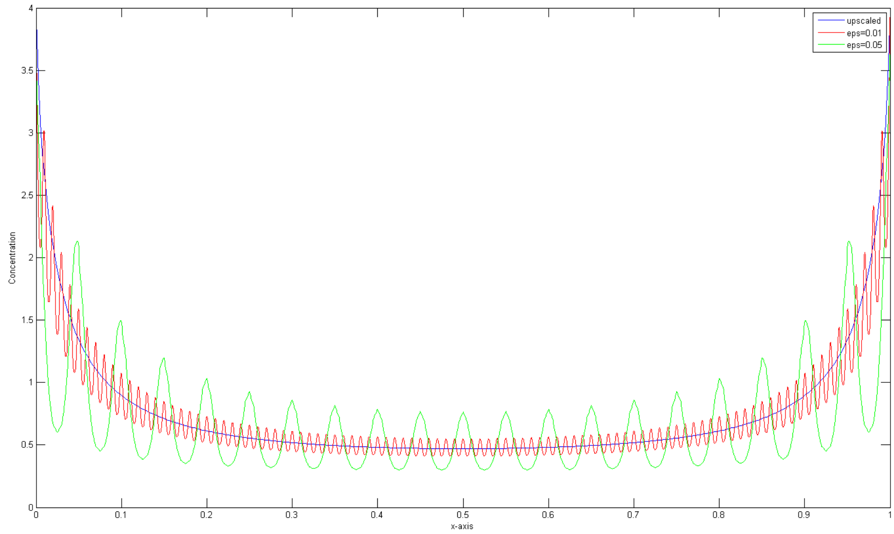

Figure 6.8: Concentrations of v^{ε} for $\varepsilon = 0.01$ and $\varepsilon = 0.05$, and v on the boundary, where $Da = 1, k = 10$.

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i	1	2	3	4	5	6
ε_i	0.1000	0.0500	0.0400	0.0250	0.0200	0.0100
$E_{\varepsilon_i}^{v_{bdry}}$	0.4642	0.3955	0.3653	0.2937	0.2569	0.1891
γ_i	-	0.2310	0.3559	0.4642	0.6000	0.4417

Table 6.9: Table for L^2 error for the adsorbent v, where $Da = 1, k = 10$.

6.2.3 Conclusion

When we choose $Da = k = 1$ our results match our expectations, the convergence orders for u^ε in the domain and u^ε and v^ε on the boundary are very close to 1, which we would expect.
We also find that when we take the Damkohler number Da larger, this has little influence on the outcome with respect to convergence orders. However, when we take constant k larger, the convergence order becomes significantly smaller.

7 Conclusions and outlook

We will kick off this concluding chapter by summarizing the results we obtained in our research up to this point. In particular, the results that are not found elsewhere in the listed literature.
There are also still some open issues left, that we will shortly mention and could serve as a topic for future research. When applicable, we will also provide possible strategies that we found and could overcome the issue. Some ideas are not carried out due to time limitations, others were unsuccessful.

7.1 Conclusion

We have derived the upscaled model for the linear adsorption desorption model that was defined in a domain with an oscillatory boundary with period and amplitude ε. This upscaled model is obtained as the limit of a sequence where $\varepsilon \searrow 0$. The derivation of this upscaled model uses homogenization arguments, the desired compactness arguments are achieved through periodic unfolding techniques. These techniques can not only be used in our linear model, but can be extended to models with non-linear - and even multi-valued - reaction rates.
We have provided numerical computations to show the convergence. We see that in general the upscaled solutions approximate the full solution very well, which shows the usefulness of the used upscaling techniques.

7.2 Outlook

The suggested geometry is relative simple but nonetheless representative. In reality, boundaries can be rough and hence not be described by a periodic function. Applying a similar upscaling procedure in a realistic geometry remains a challenge.
We found that the constants in the adsorption desorption model can be influencing the convergence order greatly. Further investigation of the effects of altering the constants is a remaining task.

Since we used COMSOL for numerical computations, we were bound by the implemented methods by COMSOL. It remains subject of investigation to find the most suitable method for solving problems like ours numerically.

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