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Bachelor Thesis

A Finite Element Method for the Numerical Simulation of Combustion

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I hereby declare that, to the best of my knowledge, this thesis is the product of my own independent work. All content and ideas drawn from external sources, directly or indirectly, published or unpublished, are indicated as such. This thesis has neither been previously submitted in whole, nor in parts, for a degree at this or any university.

Göttingen, April 3^{rd}, 2013

Signature

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Nomenclature

α	Heat transfer coefficient between gaseous and solid phase	$[\frac{W}{m^2 \cdot K}]$
ν	Velocity of the gaseous mixture	$[\frac{m}{s}]$
ρ_F	Mass density of the fuel	$[\frac{kg}{m^3}]$
ρ_G	Mass density of the gaseous mixture	$[\frac{kg}{m^3}]$
A	Pre-exponential factor	$[\frac{kg_i}{mol}]$
C_s^p	Specific heat capacity of the solid phase for constant pressure	$[\frac{J}{kg \cdot K}]$
D_g	Diffusion coefficient for the gaseous phase	$[\frac{1}{s}]$
D_s	Diffusion coefficient for the solid phase	$[\frac{m^2}{s}]$
E	Activation energy	$[\frac{J}{mol}]$
f	Measure of the residual energy fraction in the fuel	$[-]$
LCV	Lower calorific value of the fuel	$[\frac{J}{kg}]$
p	Pressure	$[P]$
R	Universal gas constant	$[\frac{J}{mol \cdot K}]$
S_V	Specific surface area of a fuel particle	$[\frac{m^2}{m^3}]$
t	Independent time variable	[s]
T_F	Temperature of the fuel	$[K]$
T_G	Temperature of the gaseous mixture	$[K]$
x	Independent spatial variable	[m]
Y_i	Mass fraction of the chemical species i	$[\frac{kg_i}{kg}]$

CHAPTER 1

Introduction

Objective Target

The topic of the thesis at hand are semilinear parabolic partial differential equations of the general format

$$\frac{\partial u}{\partial t} + \nu \frac{\partial u}{\partial x} = \delta \frac{\partial^2 u}{\partial x^2} - \mathcal{R}(u)$$

with initial conditions

$$u(x, 0) = u_0(x)$$

and constant Dirichlet boundary conditions

$$u(0, t) = \eta, \qquad u(1, t) = \beta$$

that do not necessarily have to be homogeneous. One key aspect shall be the treatment of the nonlinear reaction term $\mathcal{R}$, and an attempt will be made to explain a particular way to obtain an approximated numerical solution based on a semidiscrete Galerkin finite element method for a system of such equations representing chemical combustion.

Procedural Method

Starting with some theoretical basics, Chapter 2 will provide the tools necessary to carry out the numerical procedure, e.g. integration by parts, Sobolev spaces and the notion of weak solutions and it will introduce the variational formulation of a model equation. On the basis of the variational formulation, Chapter 3 describes the chosen method of numerical approximation by first discretizing in space using a Galerkin ansatz and then solving the problem that is still continuous in time. Additionally, two important examples of the model equation and their numerical solution implemented in MATLAB will be given. Chapter 4 contains the principal result, first specifying a brief review of the underlying model and subsequently applying the previously derived methods in order to solve the model numerically. And finally, the nonlinear model equations for combustion will be solved with this procedure and the result will be visualized and briefly discussed.

CHAPTER 2

Theoretical Fundamentals

This chapter is dedicated to providing the theoretical background for the thesis and is divided into two sections. The first will obtain basic function spaces and explain the *integration by parts* formula, whilst the second deals with partial differential equations and specifies definitions like *Lebesgue* and *Sobolev* spaces and introduces the *variational formulation* as a fundamental aspect of the numerical approximation to be conducted later.

2.1 Calculus

Firstly, a few selected function spaces will be introduced, namely, the sets of *continuous* and *continuous differentiable* functions. These spaces are going to be needed on various occasions throughout the whole thesis. Moreover, basic theorems will be given that aim to make a connection between integration and differentiation.

Definition 2.1

Let $k \in \mathbb{N} \cup \{\infty\}$.

(1) $\mathscr{C}(\Omega) := \{u \colon \Omega \subseteq \mathbb{R} \to \mathbb{R}$ *such that* u *is continuous on* $\Omega\}$

(2) $\mathscr{C}^k(\Omega) := \{u \colon \Omega \subseteq \mathbb{R} \to \mathbb{R}$ *such that* u *is* k*-times continuous differentiable on* $\Omega\}$

If the function in question is vector-valued, the codomain will be added to the name of the particular function space, e.g. a continuous function $u \colon \Omega \subseteq \mathbb{R} \to \mathbb{R}^d$ belongs to $\mathscr{C}(\Omega; \mathbb{R}^d)$. Furthermore, the *support* of a function $u \colon \Omega \subseteq \mathbb{R} \to \mathbb{R}$ is defined as $\operatorname{supp}(u) := \overline{\{x \in \Omega : u(x) \neq 0\}}$ and therefore $\mathscr{C}_c^k(\Omega) := \{u \in \mathscr{C}^k(\Omega) : \operatorname{supp}(u) \Subset \Omega\}$, whilst $\Subset$ means it is a compact subset. Functions of the type $u \in \mathscr{C}_c^\infty(\Omega)$ are called *test functions*.

The next step is to obtain a suitable method for the integration of a product of certain functions. In order to accomplish this, the following theorem will provide the tool to prove the necessary theorem.

Theorem 2.2 (*Fundamental theorem of calculus*)

Let $[a, b] \subseteq \mathbb{R}$ and $f \colon [a, b] \to \mathbb{R}$ be continuous. If a differentiable function $F \colon [a, b] \to \mathbb{R}$ exists such that $F' = f$, then $\int_a^b f(x) = F(b) - F(a)$ holds true.

Proof: Cf., for example, [Rud76, p.134, Theorem 6.21].[1] □

In the following section it will be necessary to integrate a product of functions with derivatives that occur and the subsequent theorem enables us to tentatively replace such an expression with a more pleasant one.

Theorem 2.3 (*Integration by parts*)

Let $f, g\colon [a,b] \subseteq \mathbb{R} \to \mathbb{R}$ be continuous differentiable functions on (a,b) with derivatives f' and g', then:

$$\begin{aligned} \int_a^b f'(x)g(x)\,dx &= [f(x)g(x)]_a^b - \int_a^b f(x)g'(x)\,dx \\ &:= f(b)g(b) - f(a)b(a) - \int_a^b f(x)g'(x)\,dx \end{aligned} \tag{2.1}$$

Proof: Define the function $h(x) := f(x)g(x)$ and apply the product rule $(f \cdot g)' = f' \cdot g + f \cdot g'$.

$$\begin{aligned} \Rightarrow \int_a^b f'(x)g(x)\,dx &= -\int_a^b f(x)g'(x)\,dx + \int_a^b h'(x)\,dx \\ &\overset{\text{Thm.(2.2)}}{=} -\int_a^b f(x)g'(x)\,dx + h(b) - h(a) \\ &= -\int_a^b f(x)g'(x)\,dx + [f(x)g(x)]_a^b \end{aligned}$$

The use of the fundamental theorem is valid, since the product of two differentiable functions is differentiable and, consequently, continuous as well. □

2.2 Partial Differential Equations

Partial differential equations (PDEs) are the main subject of the thesis at hand. Hence, firstly, this section will specify a few definitions, in order to be able to move swiftly to more special, and particularly, more relevant cases; namely, a *model PDE* will be given. For this type of equation, the third part of Section 2.2 provides the theoretical "scaffolding" for the posterior following numerical approximation procedure.

In addition to the already established spaces, we need the following function spaces in order to work with PDEs.

[1] In this reference, the fundamental theorem illustrates the more general case of Riemann-integrable functions. But according to [Rud76, pp.125-126, Theorem 6.8], every continuous function is Riemann-integrable and hence the above stated theorem holds true as well.

Definition 2.4 (*Lebesgue spaces $\mathscr{L}^p(\Omega)$*)

Let Ω be a Lebesgue measurable set and $p \in [1, \infty]$:

$$\mathscr{L}^p(\Omega) := \left\{ u \colon \Omega \to \mathbb{R} \text{ measurable} : ||u||_{\mathscr{L}^p(\Omega)} < \infty \right\},$$

where the norm $|| \cdot ||_{\mathscr{L}^p(\Omega)}$ is defined as

$$||u||_{\mathscr{L}^p(\Omega)} := \begin{cases} \left(\int_\Omega |u(x)|^p \, dx \right)^{\frac{1}{p}}, & p \in [1, \infty) \\ \operatorname*{ess\,sup}_{x \in \Omega} |u(x)|, & p = \infty. \end{cases}$$

The following theorem states a very imporatant fact about Lebesgue spaces.

Theorem 2.5 (*Banach space property*)

The spaces $\left(\mathscr{L}^p(\Omega), || \cdot ||_{\mathscr{L}^p(\Omega)} \right)$ are Banach spaces *wherever $p \in [1, \infty]$.*

Proof: Cf., for example, [Bre10, pp.93-94, Theorem 4.8]. □

Remark: For the special case of $p = 2$, even the space $\mathscr{L}^2(\Omega)$ with the inner product

$$\langle u, v \rangle_{\mathscr{L}^2(\Omega)} := \int_\Omega u(x) v(x) \, dx \tag{2.2}$$

is a *Hilbert space*. This inner product will be used frequently below.

2.2.1 Basic Information

As mentioned above, this section is dedicated to explaining the neccessary facts and notations concerning PDEs. As a maximum generality is not required, the following simplifications will be made.

- **Spatial univariate:** Only PDEs that are dependent of two variables need to be considered, i.e. the variable t shall denote the time dependence and x the spatial dependence.
- **Second order in space:** Let us assume that, with respect to space, there is always a differential operator of the second order assured, i.e. $\frac{\partial^2}{\partial x^2}$, since there is just one spatial variable and it is possible to have a first order operator $\frac{\partial}{\partial x}$ as well. Moreover, there are no derivatives with an order greater than two.
- **First order in time:** Concerning time, there is only the first derivative, i.e. $\frac{\partial}{\partial t}$.

Given the above restrictions, the first definition of a special PDE reads as follows.

Definition 2.6 (*Semilinear first order evolution equation*)

Let $\Omega \subseteq \mathbb{R}$ be an open interval. For $k \geq 1$, $T \in \mathbb{R}_{>0}$ and an unknown and thus sought-after function $u\colon \Omega \times (0,T) \to \mathbb{R}$, the following equation is called first order evolution equation*:*

$$\frac{\partial u}{\partial t}(x,t) - L_x u(x,t) = f(x,t), \qquad (x,t) \in \Omega \times (0,T), \tag{2.3}$$

where L_x denotes an operator of the following format:

$$L_x u(x,t) := A\left[\partial_{xx} u, \partial_x u, x, t\right] + B\left[u, x, t\right]$$

In the above equation, A and B are mappings that depend on the second and the first derivative respectively, and on u itself and the domain $\Omega \times (0,T)$. Henceforth, we will only consider the following setting: A is linear with respect to the second derivative and B can be arbitrary. For this selection of coefficient functions, the PDE (2.3) is semilinear*.*

In reality, in most situations it is very difficult to come up with a solution for a PDE with the classical concept of derivatives. Thus, let us consider extenuated derivatives with respect to space in the following manner[2].

Definition 2.7 (*Weak derivatives*)

Let $\Omega \subseteq \mathbb{R}$ be an open interval. For $k \in \mathbb{N}_0$, a function $w \in \mathscr{L}^1_{loc}(\Omega) := \{w \in \mathscr{L}^1(\Omega') : \Omega' \Subset \Omega\}$ is called the k^{th} weak derivative *of $u \in \mathscr{L}^1_{loc}(\Omega)$, if*

$$\int_\Omega u(x) \frac{d^k v}{dx^k}(x)\, dx = (-1)^k \int_\Omega w(x) v(x)\, dx \qquad \forall\ v \in \mathscr{C}^\infty_c(\Omega)$$

holds true, and will thus be denoted $\frac{d^k u}{dx^k} := w$.

Next, a model PDE that specifies exactly the type of equations to be dealt with will be given.

2.2.2 Model PDE

The aim of this thesis is to explain a way to simulate chemical reactions; thus, Definition 2.6 can be restricted. It will therefore be sufficient to consider PDEs of the following type exclusively. Let $(0,X) =: \Omega \subseteq \mathbb{R}$ be an open interval, $X > 0$, $T > 0$, $\nu > 0$, $\eta \in \mathbb{R}$, $\beta \in \mathbb{R}$ and

[2]For extenuated derivatives with respect to time, cf. section 2.2.3.

$\delta > 0$.

$$\boxed{\begin{aligned} \frac{\partial u}{\partial t}(x,t) + \nu \frac{\partial u}{\partial x}(x,t) &= \delta \frac{\partial^2 u}{\partial x^2}(x,t) - \mathcal{R}(u,x,t) && \text{in } \Omega \times (0,T) && \text{(2.4a)} \\ u(0,t) = \eta,\ u(X,t) &= \beta && \text{for } t \in [0,T] && \text{(2.4b)} \\ u(x,0) &= u_0(x) && \text{for } x \in \overline{\Omega} && \text{(2.4c)} \end{aligned}}$$

In this equation, $\mathcal{R}\colon \mathbb{R} \times \Omega \times (0,T) \to \mathbb{R}$ denotes either a loss or growth of the quantity u and may be nonlinear as well. Furthermore, the values η, β and the function $u_0 \in \mathscr{L}^2(\Omega)$ are given. Note that the so-called *Dirichlet boundary values* (2.4b) and *initial values* (2.4c) appeared for the first time here and were not mentioned in the basic information in Section 2.2.1. Nevertheless, both will be needed in order to work with the *initial boundary value problem (IBVP)* (2.4) as a special case of a so-called *parabolic* PDE. A reasonable demand on a PDE like (2.4) is that initial and boundary values agree with each other at their common points, i.e. $u_0(0) = \eta,\ u_0(1) = \beta$.

2.2.3 Variational Formulation

This section follows the notion of [GR07, pp.317-319] and [KA03, pp.288-290] and is extended and adjusted to our univariate model PDE (2.4). In order to apply the numerical procedure, the first aim is to obtain the *variational formulation* of a PDE, which mainly uses the idea of weak derivatives in a more precise modality. The first step is to multiply the equation (2.4a) itself by an arbitrary test function $v \in \mathscr{C}_c^\infty(\Omega)$ that is not time-dependent and integrate over the whole interval Ω using integration by parts:

$$\begin{aligned} \int_\Omega \frac{\partial u}{\partial t}(x,t)v(x)\,dx &= -\nu \int_\Omega \frac{\partial u}{\partial x}(x,t)v(x)\,dx + \delta \int_\Omega \frac{\partial^2 u}{\partial x^2}(x,t)v(x)\,dx - \int_\Omega \mathcal{R}(u,x,t)v(x)\,dx \\ &\overset{(2.1)}{=} -\nu \int_\Omega \frac{\partial u}{\partial x} v\,dx + \delta \left[\left[v \frac{\partial u}{\partial x} \right]_a^b - \int_\Omega \frac{\partial u}{\partial x}\frac{\partial v}{\partial x}\,dx \right] - \int_\Omega \mathcal{R}(u,x,t)v\,dx \\ &= -\nu \int_\Omega \frac{\partial u}{\partial x} v\,dx - \delta \int_\Omega \frac{\partial u}{\partial x}\frac{\partial v}{\partial x}\,dx - \int_\Omega \mathcal{R}(u,x,t)v\,dx \qquad \forall\ v \in \mathscr{C}_c^\infty(\Omega) \end{aligned} \tag{2.5}$$

Note that the above equation holds true because functions in $\mathscr{C}_c^\infty(\Omega)$ vanish at the boundary of the domain, i.e. for $\partial\Omega = \{0, X\}$. Additionally, we need to specify a space for a solution u of (2.5). Therefore, the space $H^1(\Omega)$ will be introduced as a representative of the very widely used concept of *Sobolev spaces*.

Definition 2.8 (*Sobolev space* $H^1(\Omega)$)

Let $\Omega = (0, X)$ for $X > 0$. One defines the space

$$H^1(\Omega) := \{u \in \mathscr{L}^2(\Omega) : u \text{ exhibits a weak derivative } u' \in \mathscr{L}^2(\Omega)\}.$$

A norm on this space is given by

$$||u||_{H^1(\Omega)} := \left(||u||^2_{\mathscr{L}^2(\Omega)} + ||u'||^2_{\mathscr{L}^2(\Omega)}\right)^{\frac{1}{2}}.$$

Moreover, the space $H^1_0(\Omega)$ is defined as the closure of $\mathscr{C}^\infty_c(\Omega)$ in $H^1(\Omega)$ and it is possible to prove that $\mathscr{C}^\infty_c(\Omega)$ is dense in $H^1_0(\Omega)$. Referring to [Sal08, pp.395-396, Theorem 7.4 and Proposition 7.8], $H^1(\Omega)$ is continuously embedded in $\mathscr{L}^2(\Omega)$. In dependence on the $\mathscr{L}^p$ spaces, the next theorem states a nice property of this new space.

Theorem 2.9 (*Hilbert space property*)

The space $H^1(\Omega)$ is equipped with the inner product

$$\langle u, v\rangle_{H^1(\Omega)} := \langle u, v\rangle_{\mathscr{L}^2(\Omega)} + \langle u', v'\rangle_{\mathscr{L}^2(\Omega)} = \int_0^X [u(x)v(x) + u'(x)v'(x)]\, dx$$

a Hilbert space.

Proof: Cf., for example, [Bre10, pp.203-204, Proposition 8.1]. □

With this in mind we return to (2.5) and understand $u(x,t)$ for every fixed $t \in [0,T]$ as the composition $x \mapsto u(x,t) = [\mathcal{U}(t)](x)$, where $\mathcal{U}\colon [0,T] \to H^1(\Omega)$. Note that the image of the mapping $t \mapsto \mathcal{U}(t)$ is a function in the Hilbert space $H^1(\Omega)$. Based on the idea of weak spatial derivatives in Definition 2.7, we also need a similar weakening for the occuring time-dependent derivative on the left hand side of (2.5). The space in which such a *generalized time derivative* is contained is defined as

$$\mathscr{L}^2(0,T;B) := \left\{\mathcal{U}\colon (0,T) \to X \text{ such that } \|\mathcal{U}\|_{\mathcal{L}^2(0,T;B)} := \left(\int_0^T \|\mathcal{U}(t)\|^2_B\, dt\right)^{\frac{1}{2}} < \infty\right\},$$

where B denotes a particular Banach space. Applying this idea of Banach space valued functions, the following definition shall be given:

Definition 2.10

A function $\mathcal{U} \in \mathscr{L}^2(0,T;H^1(\Omega))$ *is said to exhibit a weak (time) derivative* $\mathcal{W} \in \mathscr{L}^2(0,T;\mathscr{L}^2(\Omega))$ *if*

$$\int_0^T \mathcal{U}(t)v'(t)\,dt = -\int_0^T \mathcal{W}(t)v(t)\,dt$$

holds true for all $v \in \mathscr{C}_c^\infty(0,T)$ *and is delineated* $\mathcal{W}$ *as* $\frac{d}{dt}\mathcal{U}$.

So the precise[3] variational formulation for the generalized solution of (2.4) reads as follows.

$$\left.\begin{aligned} &\text{Find } \mathcal{U} \in \mathscr{L}^2(0,T;H^1(\Omega)) \text{ possessing } \frac{d}{dt}\mathcal{U} \in \mathscr{L}^2(0,T;\mathscr{L}^2(\Omega)) \text{ such that} \\ &\langle \frac{d}{dt}\mathcal{U}(t), v\rangle_{\mathscr{L}^2(\Omega)} + \nu\langle [\mathcal{U}(t)]', v\rangle_{\mathscr{L}^2(\Omega)} = -\delta\langle [\mathcal{U}(t)]', v'\rangle_{\mathscr{L}^2(\Omega)} - \langle \mathcal{R}(\mathcal{U}(t)), v\rangle_{\mathscr{L}^2(\Omega)} \\ &\text{holds true wherever } v \in H_0^1(\Omega) \text{ and for a.e. } t \in [0,T] \\ &\text{along with } \mathcal{U}(0) = u_0 \text{ and both } [\mathcal{U}(t)](0) = \eta \text{ and } [\mathcal{U}(t)](X) = \beta \end{aligned}\right\} \tag{2.6}$$

Based on [Eva98, pp.288-289, Theorem 4] it is possible to show that mappings $\mathcal{U} \in \mathscr{L}^2(0,T;H^1)$ with $\frac{d}{dt}\mathcal{U} \in \mathscr{L}^2(0,T;\mathscr{L}^2)$ are actually in $\mathscr{C}(0,T;\mathscr{L}^2)$ - with feasible exceptions on null sets - and hence the demand $u_0 \in \mathscr{L}^2(\Omega)$ on the initial condition (2.4c) is indeed meaningful. A closing fact about our model PDE (2.4) follows.

Theorem 2.11 (*Existence*)

Define $\Omega_T := \Omega \times (0,T)$. *Let* $\mathcal{R}$ *fulfill the following conditions:*

(1) $\mathcal{R}(s,x,t)$ *is measurable in* (x,t) *and continuous in* s

(2) $\forall\ (x,t) \in \Omega_T$ *and* $s \in \mathbb{R}\ \exists\ f \in \mathscr{L}^1(\Omega_T)$, *such that* $\mathcal{R}(s,x,t)s \geq -f(x,t)$

(3) $\forall\ r \in \mathbb{R}\ \exists\ g_r \in \mathscr{L}^1(\Omega_T)$, *such that* $\forall\ (x,t) \in \Omega_T$ *it holds* $\sup_{\|s\|\leq r} |\mathcal{R}(s,x,t)| \leq g_r(x,t)$,

then the IBVP (2.4) possesses a weak solution in the sense of (2.6) for all $u_0 \in \mathscr{L}^2(\Omega)$.

Proof: Cf., for example, [LM87, pp.33-38, Theorem 1]. Actually, the stated proof only deals with homogeneous Dirichlet data at $\partial\Omega$. However, this is not a setback since every nonhomogeneous problem can be transformed to a homogeneous one by using the mapping $\psi(x,t) := x\beta + (1-x)\eta$. Thus the theorem holds true. □

This statement concludes the theoretical background constituting the jumping-off point from which to continue with the numerical treatment in the next chapter.

[3] In fact, this is not the most general possibility to define such a variational formulation. It can be generalized by using a so-called *Gelfand triple*, which utilizes the embedding $H^1(\Omega) \subset \mathscr{L}^2(\Omega) \subset H^{-1}(\Omega)$, where H^{-1} denotes the *topological dual space* of H^1.

CHAPTER 3

Numerical Treatment

This chapter lays the foundation of the desired numerical simulation. That means that, firstly, a possibility for the approximation for the discretization in time and space of the model PDE (2.4) in general will be given. After which two very important examples will be discussed and visualized. These examples will introduce the numerical treatment of simulating certain chemical reactions and will reoccur, though in a slightly altered shape, in Chapter 4.

3.1 Method of Lines

This section follows the notion of [Joh87, pp.149-150], [KA03, pp.295-296] and [GR07, pp.154-155] and is again adjusted to our model PDE (2.4). Here, a approach called *method of lines (MOL)* is chosen and will be deduced from the results obtained in Chapter 2. The idea of this procedure is to separate the roles of time and space by means of first discretizing a PDE in space using in this case a finite element formulation and afterwards conducting the time discretization.

The goal is to sustain an approximated solution $\mathcal{U}_\Delta$ in a finite dimensional subspace $V_\Delta \subset H^1(\Omega)$ of the solution $\mathcal{U}$ of the variational formulation (2.6). In addition to the *ansatz space* V_Δ, a different finite dimensional subspace $W_\Delta \subseteq H_0^1(\Omega)$ that represents the test functions and is called *test space* is necessary. Hence, the semidiscrete (i.e. discretized in space and still continuous in time) analogon to the variational formulation (2.6) can be obtained with $u_{0,\Delta} \in V_\Delta$ as an approximation of the initial profile in the ansatz space as follows:

$$\left.\begin{aligned} \text{Find } \mathcal{U}_\Delta \in \mathscr{L}^2(0,T;V_\Delta) \text{ possessing } \frac{d}{dt}\mathcal{U}_\Delta \in \mathscr{L}^2(0,T;\mathscr{L}^2(\Omega)) \text{ such that} \\ \langle \frac{d}{dt}\mathcal{U}_\Delta(t), v_\Delta\rangle_{\mathscr{L}^2} + \nu\langle [\mathcal{U}_\Delta(t)]', v_\Delta\rangle_{\mathscr{L}^2} = -\delta\langle [\mathcal{U}_\Delta(t)]', v_\Delta'\rangle_{\mathscr{L}^2} - \langle \mathcal{R}(\mathcal{U}_\Delta(t)), v_\Delta\rangle_{\mathscr{L}^2} \\ \text{holds true for all } v_\Delta \in W_\Delta \text{ and for a.e. } t \in [0,T] \\ \text{along with } \mathcal{U}_\Delta(0) = u_{0,\Delta} \text{ and both } [\mathcal{U}_\Delta(t)](0) = \eta \text{ and } [\mathcal{U}_\Delta(t)](X) = \beta \end{aligned}\right\} \tag{3.1}$$

Now, the objective is to achieve a more satisfactory expression for this problem relating to a numerical procedure that can be handled with existing methods. Therefore the ansatz and test spaces will be specified by supposing that $V_\Delta = \text{span}\{\psi_i\}$ and $W_\Delta = span\{\phi_i\}$ with some bases $\mathcal{A} = \{\psi_i\}$ and $\mathcal{T} = \{\phi_i\}$. Both bases $\mathcal{A}$ and $\mathcal{T}$ shall consist of piecewise linear functions

and are only different at the boundary of the considered spatial domain $\Omega = (0,1)$. For the discretization in space, divide Ω equidistantly into $n+1$ intervals of length $\Delta x := \frac{1}{n+1}$, identify the inner points by x_i for $i = 1, \dots, n$ and regard the boundary values as $x_0 := 0$ and $x_{n+1} := 1$. With the aid of this mesh, define

$$\psi_i(x) = \phi_i(x) := \begin{cases} \frac{1}{\Delta x}(x - x_{i-1}) & \text{, for} \quad x \in [x_{i-1}, x_i] \\ \frac{1}{\Delta x}(x_{i+1} - x) & \text{, for} \quad x \in (x_i, x_{i+1}] \\ 0 & \text{, else} \end{cases}$$

for the inner points $i = 1, \dots, n$. Note that the distinction between $\mathcal{A}$ and $\mathcal{T}$ for the inner points is just a formal measure. Because of the appearance of these functions (cf. Figure 3.1), they are called *hat functions*. Additionally, it is necessary to expand $\mathcal{A}$ with the correspondent functions $\psi_0(x) := \frac{1}{\Delta x}(x_1 - x)\mathbf{1}_{[0,x_1]}(x)$ and $\psi_{n+1}(x) := \frac{1}{\Delta x}(x - x_n)\mathbf{1}_{[x_n,1]}(x)$, where $\mathbf{1}$ represents the *indicator function*, since the model PDE (2.4) allows nonhomogeneous Dirichlet conditions.

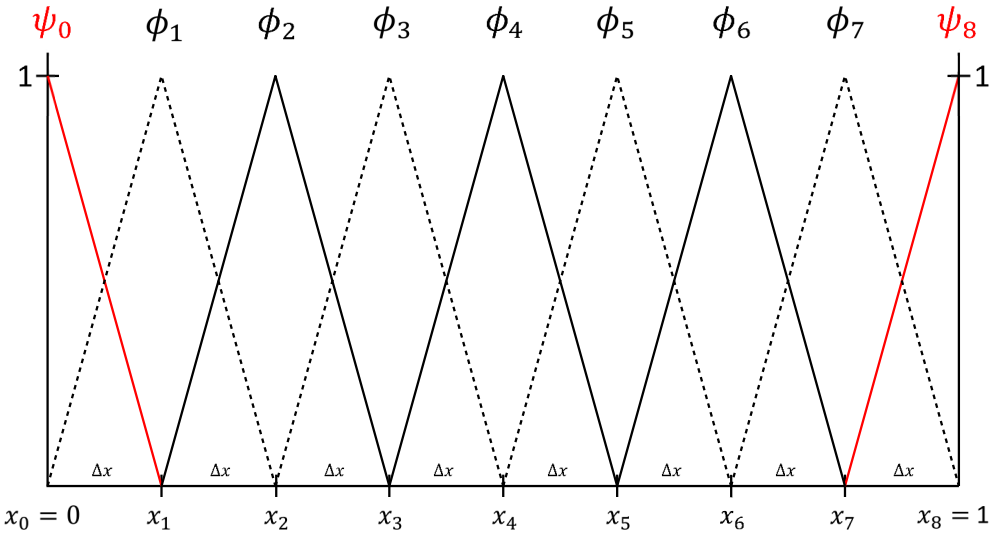


Figure 3.1: Ansatz and Test Functions for $n = 7$

Futhermore, note that in the sense of weak derivatives

$$\psi_i'(x) = \phi_i'(x) = \begin{cases} \frac{1}{\Delta x} & \text{, for} \quad x \in [x_{i-1}, x_i] \\ -\frac{1}{\Delta x} & \text{, for} \quad x \in (x_i, x_{i+1}] \\ 0 & \text{, else} \end{cases}$$

is the first derivative of the i-th hat function $\psi_i = \phi_i$ for $i = 1, \dots, n$ and analogously $\psi_0'(x) = -\frac{1}{\Delta x}\mathbf{1}_{[0,x_1]}(x)$ and $\psi_{n+1}'(x) = \frac{1}{\Delta x}\mathbf{1}_{[x_n,1]}(x)$. Hence, altogether, we can observe that $\text{span}\{\psi_0, \dots, \psi_{n+1}\} = V_\Delta \subseteq H^1(\Omega)$ and $\text{span}\{\phi_1, \dots, \phi_n\} = W_\Delta \subseteq H_0^1(\Omega)$, which makes it viable to specify the approximation in (3.1) as a linear combination of functions in $\mathcal{A}$ as

$\mathcal{U}_\Delta(t) := \sum_{j=0}^{n+1} y_j(t)\psi_j$. The aim is to find the unknown functions $y_j(t)$ which represent the values of the approximated solution. Actually, we already know what values the solution has to attain at the boundary of the spatial domain, as they were fixed within the formulation for the model PDE (2.4) as $y_0(t) = \eta$ and $y_{n+1}(t) = \beta$ for any $t \in [0, T]$, hence we can circumstantiate the approximation as follows:

$$\mathcal{U}(t) \approx \mathcal{U}_\Delta(t) := \eta\psi_0 + \sum_{j=1}^{n} y_j(t)\psi_j + \beta\psi_{n+1} \tag{3.2}$$

With the selection of $v_h = \phi_i$ for $i = 1, \ldots, n$ as test functions, the following calculation shows that the formulation (3.1) is equivalent to a system of initial value problems for *ordinary differential equations (ODEs)* which can be solved by well-known procedures like *Runge-Kutta, Euler or Crank-Nicolson.* Thus, inserting (3.2) into the semidiscrete equation (3.1) results in the following equation for $i = 1, \ldots, n$.

$$\begin{aligned}
&\int_\Omega \frac{\partial}{\partial t}\left[\eta\psi_0 + \sum_{j=1}^{n} y_j(t)\psi_j + \beta\psi_{n+1}\right]\phi_i(x)\,dx + \nu\int_\Omega \frac{\partial}{\partial x}\left[\eta\psi_0 + \sum_{j=1}^{n} y_j(t)\psi_j + \beta\psi_{n+1}\right]\phi_i(x)\,dx \\
&\qquad = -\delta\int_\Omega \frac{\partial}{\partial x}\left[\eta\psi_0 + \sum_{j=1}^{n} y_j(t)\psi_j + \beta\psi_{n+1}\right]\frac{\partial}{\partial x}\phi_i(x)\,dx - \int_\Omega \mathcal{R}(\mathcal{U}_\Delta(x,t))\phi_i\,dx
\end{aligned}$$

Taking into account that both integration and derivation are linear, and that integration only depends on space where $y_i(t)$ only depends on time, one obtains:

$$\begin{aligned}
&\sum_{j=1}^{n}\left[\frac{dy_j}{dt}(t)\int_\Omega \psi_j(x)\phi_i(x)\,dx\right] + \nu\sum_{j=1}^{n}\left[y_j(t)\int_\Omega \psi_j'(x)\phi_i(x)\,dx\right] \\
&\quad + \nu\left[\eta\int_\Omega \psi_0'(x)\phi_i(x)\,dx + \beta\int_\Omega \psi_{n+1}'(x)\phi_i(x)\,dx\right] \\
&\quad = -\delta\sum_{j=1}^{n}\left[y_j(t)\int_\Omega \psi_j'(x)\phi_i'(x)\,dx\right] - \int_\Omega \mathcal{R}(\mathcal{U}_\Delta(x,t))\phi_i\,dx \\
&\quad + \delta\left[\eta\int_\Omega \psi_0'(x)\phi_i'(x)\,dx + \beta\int_\Omega \psi_{n+1}'(x)\phi_i'(x)\,dx\right], \qquad i = 1, \ldots, n
\end{aligned}$$

Written with the inner product $\langle\cdot,\cdot\rangle_{\mathscr{L}^2(\Omega)}$:

$$\begin{aligned}
\sum_{j=1}^{n}\langle\psi_j, \phi_i\rangle_{\mathscr{L}^2}\frac{d}{dt}y_j(t) = &-\nu\sum_{j=1}^{n}\langle\psi_j', \phi_i\rangle_{\mathscr{L}^2}y_j(t) - \delta\sum_{j=1}^{n}\langle\psi_j'(x), \phi_i'\rangle_{\mathscr{L}^2}y_j(t) - \delta\langle\eta\psi_0' + \beta\psi_{n+1}', \phi_i'\rangle_{\mathscr{L}^2} \\
&- \nu\langle\eta\psi_0' + \beta\psi_{n+1}', \phi_i\rangle_{\mathscr{L}^2} - \int_\Omega \mathcal{R}(\mathcal{U}_\Delta(x,t))\phi_i\,dx, \qquad i = 1, \ldots, n
\end{aligned}$$

To complete the ODE problem, the inital values for the vector $y(t)$ are required. So the

condition (2.4c) has to be approximated appropriately, which can be done by

$$u_0(x) \approx u_{0,\Delta}(x) = \eta\psi_0 + \sum_{j=1}^{n} \alpha_j \psi_j + \beta\psi_0,$$

in which the coefficients α_j have to be chosen such that $\|u_{0,\Delta} - u_0\|_{\mathscr{L}^2(\Omega)} \to 0$ for $n \to \infty$[4]. Actually, the above computation just considers the inner points $x_1, \ldots, x_n$. In order to take account of the boundary points, the two ODEs $y_0'(t) = 0$ with $y_0(0) = \eta$ and $y_{n+1}'(t) = 0$ with $y_{n+1}(0) = \beta$ have to be added for x_0 and x_{n+1}, respectively, since the values of the solution are not supposed to change during the contemplated time period $[0, T]$. For the time being[5], let $\mathcal{R} \equiv 0$. If so, the semidiscrete variational formulation can be written modestly in matrix-vector form as

$$\boxed{\begin{aligned} M\frac{d}{dt}y(t) &= -\left[\nu C + \delta D\right] y(t) - \left[\nu b^c + \delta b^d\right] && \text{(3.3a)} \\ y(0) &= (\alpha_i)_{0\le i\le n+1} && \text{(3.3b)} \end{aligned}}$$

with $\alpha_0 = \eta$, $\alpha_{n+1} = \beta$ and $M, C, D \in \mathbb{R}^{(n+2)\times(n+2)}$ matrices given by

$$M := \begin{pmatrix} 1 & 0 & \cdots & 0 \\ \mathbf{0} & \left(\langle \psi_j, \phi_i \rangle_{\mathscr{L}^2}\right)_{1\le i,j\le n} & & \mathbf{0} \\ 0 & \cdots & 0 & 1 \end{pmatrix}, \; C := \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \mathbf{0} & \left(\langle \psi_j', \phi_i \rangle_{\mathscr{L}^2}\right)_{1\le i,j\le n} & & \mathbf{0} \\ 0 & \cdots & 0 & 0 \end{pmatrix},$$

$$D := \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \mathbf{0} & \left(\langle \psi_j', \phi_i' \rangle_{\mathscr{L}^2}\right)_{1\le i,j\le n} & & \mathbf{0} \\ 0 & \cdots & 0 & 0 \end{pmatrix}$$

and $y(t), b^c, b^d \in \mathbb{R}^{n+2}$ vectors given by:

$$y(t) := \begin{pmatrix} y_0(t) \\ y_1(t) \\ \vdots \\ y_n(t) \\ y_{n+1}(t) \end{pmatrix}, \qquad b^c := \begin{pmatrix} 0 \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_1 \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix}, \qquad b^d := \begin{pmatrix} 0 \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_1' \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_n' \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix}$$

Note that $\mathbf{0} \in \mathbb{R}^n$ denotes the n-dimensional zero vector. In order to improve the comprehensibility of this procedure and, particularly, its name, consider Figure 3.2 which visualizes the above introduced MOL.

[4] An example for such an approximation is simply to evaluate the initial profile pointwise.
[5] Handling nonlinear reaction terms will be the main subject later, in concrete situations.

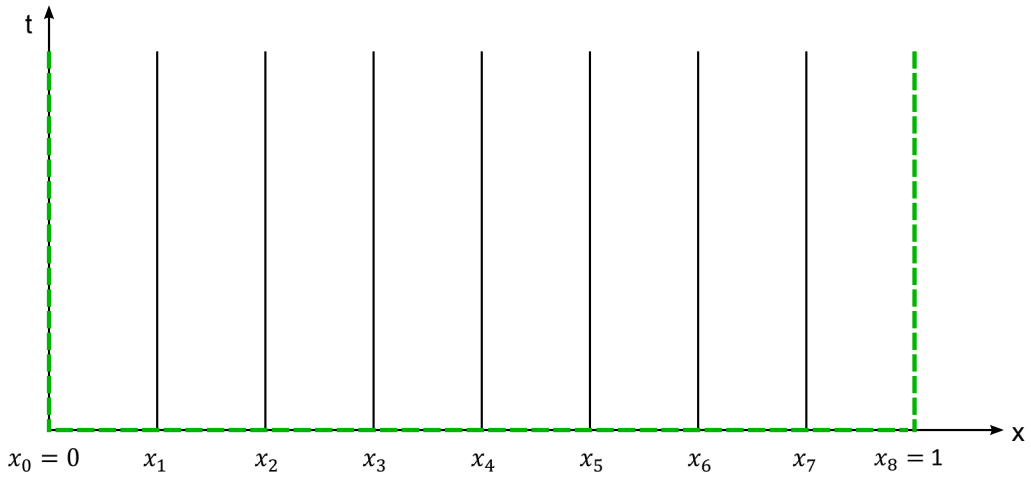


Figure 3.2: Method of Lines Visualization for $n = 7$

The MOL starts by discretizing a PDE with respect to space only. This can be seen in Figure 3.2 as dividing the originally continous spatial domain $(0, 1)$ into several intervals. Mathematically, this means that the underlying PDE has been transformed into a system of exactly that number of ODEs of the quantity of spatial subdivisions. We know both the initial and the boundary conditions illustrated as dashed green lines in Figure 3.2. We only have to solve for the inner values illustrated as black lines in Figure 3.2. Note that if the original PDE has, for example, nonlinear reaction terms, then the ODE system will also be nonlinear.

The next objective is to obtain a more specific form for the required matrices M, C and D and the vectors b^c and b^d in (3.3). Hence, the following integrals of these hat functions have to be computed and the values obtained will be used excessively later on.

$$m_{ij} := \langle \psi_j, \phi_i \rangle_{\mathscr{L}^2(\Omega)} = \int_0^1 \psi_j(x)\phi_i(x)\,dx \Rightarrow M^* := (m_{ij})_{1\le i,j\le n} = \Delta x \ \text{tridiag}\left(\frac{1}{6}, \frac{2}{3}, \frac{1}{6}\right)$$

$$c_{ij} := \langle \psi_j', \phi_i \rangle_{\mathscr{L}^2(\Omega)} = \int_0^1 \psi_j'(x)\phi_i(x)\,dx \Rightarrow C^* := (c_{ij})_{1\le i,j\le n} = \text{tridiag}\left(-\frac{1}{2}, 0, \frac{1}{2}\right)$$

$$d_{ij} := \langle \psi_j', \phi_i' \rangle_{\mathscr{L}^2(\Omega)} = \int_0^1 \psi_j'(x)\phi_i'(x)\,dx \Rightarrow D^* := (d_{ij})_{1\le i,j\le n} = \frac{1}{\Delta x}\ \text{tridiag}\,(-1, 2, -1)$$

For $a, b, c \in \mathbb{R}$ the expression $\text{tridiag}(a, b, c)$ shall describe the matrix comprising the numbers a, b, c as sub-, main- and superdiagonal respectively. Thus, note that the matrices $M, C, D \in \mathbb{R}^{(n+2)\times(n+2)}$ are all sparse because the hat functions have a very small support, namely $supp\,(\psi_i \cdot \phi_j) = \emptyset \Leftrightarrow |i-j| \ge 2$. This fact can also be used very effectively to recognize

that the following vectors to have only two non-zero elements in case of $\eta, \beta \neq 0$.

$$b^c := \begin{pmatrix} 0 \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_1 \rangle_{\mathscr{L}^2} \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_{n-1} \rangle_{\mathscr{L}^2} \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta\langle \psi_0', \phi_1 \rangle_{\mathscr{L}^2} \\ 0 \\ \vdots \\ 0 \\ \beta\langle \psi_{n+1}', \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} 0 \\ -\eta \\ 0 \\ \vdots \\ 0 \\ \beta \\ 0 \end{pmatrix}$$

$$b^d := \begin{pmatrix} 0 \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_1' \rangle_{\mathscr{L}^2} \\ \langle \eta\phi_0' + \beta\phi_{n+1}', \phi_2' \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_{n-1}' \rangle_{\mathscr{L}^2} \\ \langle \eta\psi_0' + \beta\psi_{n+1}', \phi_n' \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta\langle \psi_0', \psi_1' \rangle_{\mathscr{L}^2} \\ 0 \\ \vdots \\ 0 \\ \beta\langle \psi_{n+1}', \psi_n' \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \frac{1}{\Delta x} \begin{pmatrix} 0 \\ -\eta \\ 0 \\ \vdots \\ 0 \\ -\beta \\ 0 \end{pmatrix}$$

3.2 Selected Examples

Let $\Omega = (0, 1)$ again. The method of lines shall be based upon $\mathcal{A}$ and $\mathcal{T}$ as bases for the ansatz and test space respectively. The major reason for studying these examples is the notion that their analysis might be able to provide a fundamental unterstanding of how to advance with the construction of an MOL procedure for modeling in Chapter 4. The first one is a simple diffusion equation without any reaction terms. Diffusion, incorporated with a second spatial derivative, is one of the most important phenomena occuring in the later simulation and this is, along with the need to become accustomed to the procedure described in Section 3.1, the reason for giving this example. The second one is mainly designed for a different purpose. In order to assemble the ODE system (3.3), we assumed no reaction to be present, i.e. $\mathcal{R} \equiv 0$. Section 3.2.2 deals with a special case of $\mathcal{R} \not\equiv 0$ that will reoccur in Chapter 4 and even in a slightly easier form. The intention is to explain how one can handle such nonlinear reaction terms, and additionally, there will be a convective term, represented by a first spatial derivative, that embodies convection as the second important phenomenom of the simulation.

3.2.1 Homogeneous Heat Equation

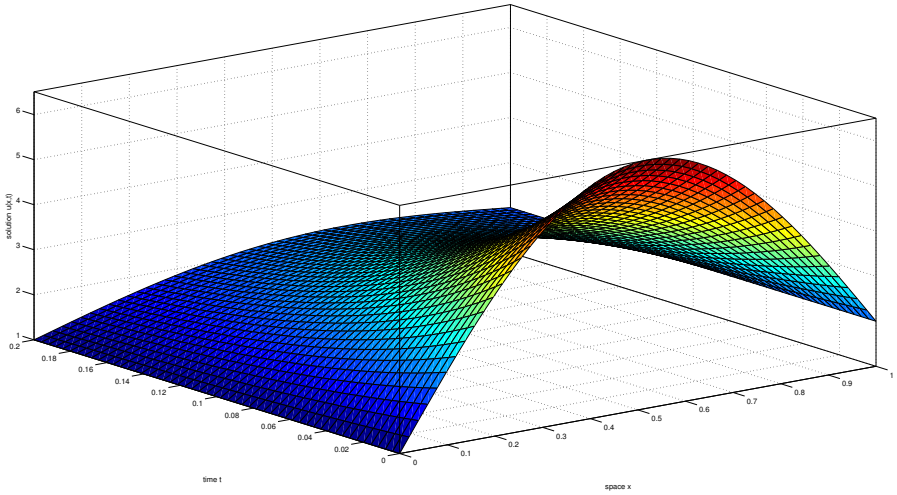
Consider the following IBVP with $\delta > 0$:

$$\boxed{\begin{aligned} \frac{\partial u}{\partial t}(x,t) &= \delta \frac{\partial^2 u}{\partial x^2}(x,t) && \text{in } \Omega \times (0,T) && \text{(3.4a)} \\ u(0,t) = 1,\ u(1,t) &= 2 && \text{for } t \in [0,T] && \text{(3.4b)} \\ u(x,0) &= 5\sin(\pi x) + x + 1 && \text{for } x \in \overline{\Omega} && \text{(3.4c)} \end{aligned}}$$

Note that we have the situation of our model PDE (2.4) with $\mathcal{R}(u) \equiv 0$, $\nu = 0$, $\eta = 1$, $\beta = 2$ and $u_0(x) = 5\sin(\pi x) + x + 1$, at which the compatibility condition is indeed fulfilled. Thus, we can assemble our ODE system $M \frac{d}{dt} y(t) = -\delta D y(t) - b^d$ and $y(0) = [5\sin(\pi x_i) + x_i + 1]_{0 \le i \le n+1}$ with the values provided by Section 3.1 as follows.

$$\Delta x \begin{pmatrix} 1 & \mathbf{0} & 0 \\ \mathbf{0} & M^* & \mathbf{0} \\ 0 & \mathbf{0} & 1 \end{pmatrix} \begin{pmatrix} \frac{d}{dt} y_0(t) \\ \frac{d}{dt} y_1(t) \\ \vdots \\ \frac{d}{dt} y_n(t) \\ \frac{d}{dt} y_{n+1}(t) \end{pmatrix} = -\frac{\delta}{\Delta x} \begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0} & D^* & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{pmatrix} \begin{pmatrix} y_0(t) \\ y_1(t) \\ \vdots \\ y_n(t) \\ y_{n+1}(t) \end{pmatrix} - \frac{\delta}{\Delta x} \begin{pmatrix} 0 \\ -1 \\ \mathbf{0} \\ -2 \\ 0 \end{pmatrix}$$

A visualization of the homogeneous heat equation (3.4) follows. The ODE system is solved with the MATLAB ODE solver *ode15s* for so-called *stiff*[6] differential equations that directly give the possibility to handle the so-called *mass matrix* M.



[6] Actually, a general definition of the term *stiff* is very difficult. Nonetheless, the impact of such a differential equation can be explained, as it is inevitable to use *implicit* methods for solving, since *explicit* ones will not function satisfactorily.

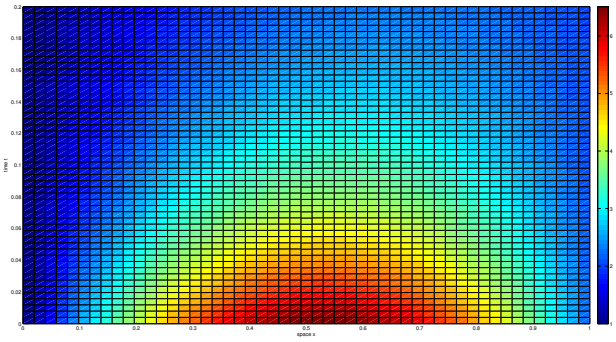


Figure 3.1: Homogeneous Heat Equation with $T = 0.2$, $n = 50$ and $\delta = 1$

3.2.2 Semilinear Convection Diffusion Reaction Equation

Let $\nu > 0$, $\delta > 0$ and $\lambda \in \mathbb{R}$.

$$\boxed{\begin{aligned} \frac{\partial u}{\partial t} + \nu \frac{\partial u}{\partial x} &= \delta \frac{\partial^2 u}{\partial x^2} - \lambda u \exp\left(-\frac{1}{u}\right) && \text{in } \Omega \times (0,T) && \text{(3.5a)} \\ u(0,t) = 2,\ u(1,t) &= 1 + \exp(-5) && \text{for } t \in [0,T] && \text{(3.5b)} \\ u(x,0) &= \exp(-5x) + 1 && \text{for } x \in \overline{\Omega} && \text{(3.5c)} \end{aligned}}$$

This is a situation similar to our model PDE (2.4) with $\mathcal{R}(u(x,t)) = \lambda u(x,t) \exp\left(-\frac{1}{u(x,t)}\right)$, $\eta = 2$, $\beta = 1 + e^{-5}$ and $u_0(x) = \exp(-5x) + 1$ at which the compatibility condition is also fulfilled. According to Section 3.1, we now want to approximate the nonlinearity in the same manner with the notion of $\mathcal{U}_\Delta(x,t) = \eta\psi_0(x) + \sum_{j=1}^n y_j(t)\psi_j(x) + \beta\psi_{n+1}(x)$. The only difference is that a nonlinear reaction term leads to a likewise nonlinear ODE system. But solving such a system is the assignment of the chosen ODE integrator, which will not be discussed here. For better lucidity, the denomination of the indepent variables (x,t) is suppressed from here on.

$$\begin{aligned} \int_\Omega \mathcal{R}(\mathcal{U}_\Delta)\phi_i \, dx =& \lambda \int_\Omega \mathcal{U}_\Delta \exp\left(-\frac{1}{\mathcal{U}_\Delta}\right) \phi_i \, dx \\ =& \lambda \int_\Omega \left[\eta\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta\psi_{n+1}\right] \exp\left(-\left[\eta\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta\psi_{n+1}\right]^{-1}\right) \phi_i \, dx \\ =& \lambda \int_\Omega \left(\sum_{j=1}^n y_j(t)\psi_j\right) \exp\left(-\left[\eta\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta\psi_{n+1}\right]^{-1}\right) \phi_i \, dx \\ &+ \lambda \int_\Omega (\eta\psi_0 + \beta\psi_{n+1}) \exp\left(-\left[\eta\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta\psi_{n+1}\right]^{-1}\right) \phi_i \, dx \\ =:& \lambda \left[I_i^c + I_i^b\right], \qquad i = 1, \ldots, n \end{aligned}$$

Now we want to consecutively analyze the two last terms in order to obtain a reasonable expression that can be appended to the ODE system (3.3). Moreover, the expressions will be carried out again with the inner product $\langle \cdot, \cdot \rangle_{\mathscr{L}^2(\Omega)}$ and directly written in vector form.

$$b^r := \begin{pmatrix} 0 \\ I_1^b \\ I_2^b \\ \vdots \\ I_{n-1}^b \\ I_n^b \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \langle \eta\psi_0 \exp\left(-\left[\eta\psi_0 + y_1(t)\psi_1\right]^{-1}\right), \phi_1 \rangle_{\mathscr{L}^2} \\ 0 \\ \vdots \\ 0 \\ \langle \beta\psi_{n+1} \exp\left(-\left[y_n(t)\psi_n + \beta\psi_{n+1}\right]^{-1}\right), \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix}$$

This computation used again that for hat functions, $supp\,(\psi_i \cdot \phi_j) = \emptyset \Leftrightarrow |i-j| \geq 2$. The last step is to treat the remaining integrals I_i^c with the same fact about the small support of products of hat functions, i.e. the vector $c^r := (I_i^c)_{1 \leq i \leq n}$ needs to be computed. For the lucidity, $y_i(t)$ will be abbreviated as simply y_i.

$$c^r = \begin{pmatrix} 0 \\ \langle (y_1\psi_1 + y_2\psi_2) \exp\left(-\left[\eta\psi_0 + y_1\psi_1 + y_2\psi_2\right]^{-1}\right), \phi_1 \rangle_{\mathscr{L}^2} \\ \langle (y_1\psi_1 + y_2\psi_2 + y_3\psi_3) \exp\left(-\left[y_1\psi_1 + y_2\psi_2 + y_3\psi_3\right]^{-1}\right), \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle (y_{n-2}\psi_{n-2} + y_{n-1}\psi_{n-1} + y_n\psi_n) \exp\left(-\left[y_{n-1}\psi_{n-2} + y_{n-1}\psi_{n-1} + y_n\psi_n\right]^{-1}\right), \phi_{n-1} \rangle_{\mathscr{L}^2} \\ \langle (y_{n-1}\psi_{n-1} + y_n\psi_n) \exp\left(-\left[y_{n-1}\psi_{n-1} + y_n\psi_n + \beta\psi_{n+1}\right]^{-1}\right), \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix}$$

Actually, it is not possible to give a cohesive expression for all of the above values of integrals. Hence, an implementation would need some numerical integration procedures to get the required values. With the introduced vectors and the grid points of the spatial discretization x_i described above, the problem (3.5) in ODE form would be written like:

$$\boxed{\begin{aligned} M\frac{d}{dt}y(t) &= -\left[\nu C + \delta D\right] y(t) - \left[\nu b^c + \delta b^d\right] - \lambda\left[b^r + c^r\right] \\ y(0) &= \left[\exp\left(-5x_i\right) + 1\right]_{0 \leq i \leq n+1} \end{aligned}}$$

The following visualization of the PDE (3.5) is obtained with the MATLAB integration routine *trapz* and the time integration is managed by the MATLAB ODE solver *ode15s*:

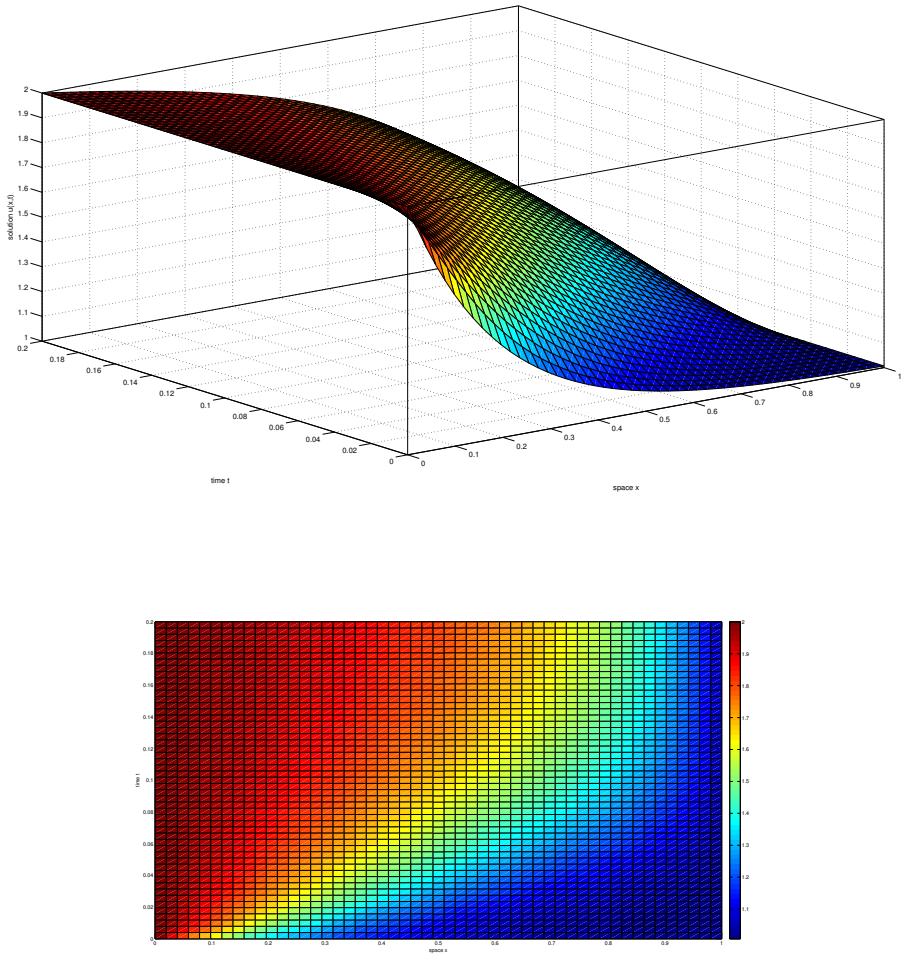


Figure 3.2: Semilinear Convection Diffusion Reaction Equation with $T = 0.2$, $n = 50$, $\nu = 5$, $\delta = 1$ and $\lambda = 1$

This concludes the introductory examples. The next chapter will follow the procedures introduced with these two PDEs, only with a slightly different reaction term $\mathcal{R}$.

CHAPTER 4

Simulating Combustion

Chapter 4 is the main body of this thesis. All of the previous results serve to explain an accurate way to obtain a numerical approximation for the following mathematical model. This approximation will be explained circumstantially and afterwards, its meaningfulness will come to light with the help of some visualizations.

4.1 Survey of the Modeling

The following simulation is predicated upon the chemical reaction

$$C + O_2 \rightarrow CO_2$$

that depicts the combustion of carbon as a solid matter with the help of pure oxygen, resulting in carbon dioxide as the reaction product. We shall use PDEs for the purpose of describing this occurrence with mathematical methods. Actually, there is the need not only to have one single PDE, but a whole system of PDEs that is to be solved simultaneously. Every part of this system specifies a certain quantity[7] that is part of both the law of conservation of mass and conservation of energy:

- Y_{O_2}: Mass fraction of the oxygen, i.e. the percentage of oxygen in the gaseous mixture that is only supposed to consist of oxygen and carbon dioxide. By virtue of this assumption, the mass fraction of the carbon dioxide can be computed easily as $Y_{CO_2} = 1 - Y_{O_2}$ and there is no need for a PDE for this factor.
- ρ_G: Mass density of the gaseous mixture.
- ρ_F: Mass density of the fuel.
- T_F: Temperature of the fuel.

The considered situation of the combustion is as follows: Assume that there is a reactor in which the fuel is located on a grid. The oxygen is able to enter the reactor near the ground, permeates the fuel in the form of carbon particles and reacts to carbon dioxide that leaves the

[7]For the completeness of the model, one can extract the particular units from the above-stated nomenclature.

reactor near the top. Furthermore, we will assume that the emerging ash is capable of falling through the grid to the bottom of the reactor. Note that only the gaseous phase moves with a certain velocity whereas the fuel is assumed to remain motionless during the whole process. A drawing[8] of the considered reactor in Figure 4.1 is shown. In addition, the modeling only takes into account a certain area of the reactor, namely the *oxidation zone*, which is emphasized by a grey rectangle. Above this combustion zone, there are other phenomena which occur like *reduction, pyrolysis* and a possible *drying* of the fuel which are not important within the framework of this simulation.

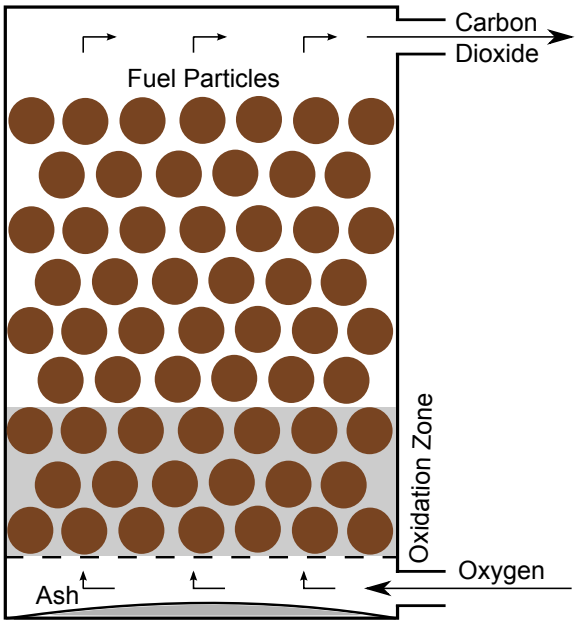


Figure 4.1: Combustion reactor

The change of a quantity in the model shall be caused by *convection, diffusion* or *reaction*, whereby each can be allocated to a particular term in our model PDE (2.4) as follows:

- The convective term is given by the first spatial derivative and its intensity can be controlled by the factor ν.
- The diffusion can be traced back to the second spatial derivative and controlled by δ.
- $\mathcal{R}$ describes certain types of reactive behaviour.

Additionally, the temporal change is to be considered as well, which is implemented in the model by the first time derivative. The complete system of equations that is to be solved will

[8] Of course, the sketch is two-dimensional in space, contrary to the assumption in Section 2.2.1 that the considered PDEs are spatial univariate. In fact, such a reactor is considerably higher to such an extent that the notion to work only in one spatial dimension is a coherent simplification.

be posed in the following way: The spatial domain shall again be the open interval $\Omega = (0, 1)$. Then the PDE (4.1) describes the change of the mass fraction of the oxygen. Thereby, $\nu > 0$ denotes the constant velocity of the oxygen flowing in, $D_g > 0$ is the diffusion coefficient for the gaseous phase, and the pre-exponential factor A, together with the exponential term of the activation energy E, the universal gas constant R and the temperature of the fuel T_F constitutes the so-called *Arrhenius term* that describes the reaction itself. The boundary conditions amount that at the bottom of the oxidation zone, there is just pure oxygen present, whereas at the top, the oxygen has completely vanished and just pure carbon dioxide is left over. Over and above an initial profile for the beginning of the simulation is given by (4.1c).

$$\frac{\partial Y_{O_2}}{\partial t} + \nu \frac{\partial Y_{O_2}}{\partial x} = D_g \frac{\partial^2 Y_{O_2}}{\partial x^2} - \left[\frac{32}{12} + Y_{O_2}\right] Y_{O_2} A \exp\left(-\frac{E}{RT_F}\right) \qquad \text{in } \Omega \times (0,T) \tag{4.1a}$$

$$Y_{O_2}(0,t) = 1 =: \eta_1,\ Y_{O_2}(1,t) = 0 \qquad \text{for } t \in [0,T] \tag{4.1b}$$

$$Y_{O_2}(x,0) = \exp^2(-1.5x) - x^{20}\exp^2(-1.5) \qquad \text{for } x \in \overline{\Omega} \tag{4.1c}$$

The next equation (4.2) in the system is actually not a PDE, but rather a simple algebraic relation deduced from the ideal gas law, and describes the mass density of the gaseous mixture ρ_G via the already described Y_{O_2}, the ambient pressure p, the universal gas constant R and the temperature of the gas T_G, which is assumed to stay constant.

$$\rho_G(x,t) = \frac{352p}{10^3 R T_g \left[3Y_{O_2}(x,t) + 8\right]}, \qquad (x,t) \in \Omega \times (0,T) \tag{4.2}$$

Furthermore, (4.3a)-(4.3c) deal with the density of the fuel and is not a classical PDE either, since there is only one partial derivative. The reason is that we have assumed that the fuel does not move at all and thus has no convective term, and, in addition, that diffusion of mass cannot happen within a solid phase. Hence the temporal and reactive changes are left. In order to include the accruement of ash, ρ_F is not allowed to reach the limit 0, or even to become negative, but the reaction is assumed to stop for locations with $\rho_F < 10$, i.e. the pre-exponential factor A is going to be zero for such a situation for every PDE involved.

$$\frac{\partial \rho_F}{\partial t}(x,t) = -\rho_G(x,t) Y_{O_2}(x,t) A \exp\left(-\frac{E}{RT_F(x,t)}\right) \qquad \text{in } \Omega \times (0,T) \tag{4.3a}$$

$$\rho_F(0,t) = 10,\ \rho_F(1,t) = 100 \qquad \text{for } t \in [0,T] \tag{4.3b}$$

$$\rho_F(x,0) = 100\sqrt{x} + 10(1-x) \qquad \text{for } x \in \overline{\Omega} \tag{4.3c}$$

Lastly, we want to consider the change of temperature of the fuel T_F in the form of the PDE (4.4) depending on time, diffusion, reaction and heat transfer between gas and fuel. Again,

there is no convective term, due to the fact that the fuel is supposed to be static. Furthermore, C_s^p denotes the specific heat capacity of the solid phase for constant pressure, D_s is the diffusion coefficient for the solid phase, S_V delineates the specific surface area of a fuel particle, α is the heat transfer coefficient, LCV specifies the lower calorific value of the fuel and f is a measure of the residual energy fraction in the fuel.

$$\frac{\partial T_F}{\partial t}(x,t) = D_s \frac{\partial^2 T_F}{\partial x^2}(x,t) + \frac{S_V \alpha}{\rho_F C_s^p}\left[T_G - T_F(x,t)\right] \tag{4.4a}$$

$$+ f\frac{\rho_G Y_{O_2}}{\rho_F C_s^p} A \exp\left(-\frac{E}{RT_F(x,t)}\right) LCV \qquad \text{in } \Omega \times (0,T) \tag{4.4b}$$

$$T_F(0,t) = 500 =: \eta_3,\ T_F(1,t) = 1500 =: \beta_3 \qquad \text{for } t \in [0,T] \tag{4.4c}$$

$$T_F(x,0) = 500 \qquad \text{for } x \in \overline{\Omega} \tag{4.4d}$$

Next, this system of equations shall be solved with the procedure introduced above.

4.2 Method of Lines for the Combustion Model

The whole discretization will use the hat functions introduced in Section 3.1 as a basis, together with $\Omega = (0,1)$ as the spatial domain of interest. This section contains the numerical approximation and consequently delivers the main results of the thesis.

4.2.1 Mass Fraction of Oxygen

The objective here is to apply the MOL to equation (4.1). Since this equation has the form of the model PDE (2.4), only the treatment of the reaction term $\mathcal{R}(Y_{O_2}) = \left[\frac{32}{12} + Y_{O_2}\right] Y_{O_2} A \exp\left(-\frac{E}{RT_F}\right)$ has to be carried out, similarly to Section 3.2.2. For better clarity, let $\lambda_i := A \exp\left(-\frac{E}{RT_{F,i}}\right)$.

$$\begin{aligned}
\int_\Omega \mathcal{R}(Y_{O_{2_\Delta}})\phi_i\,dx &= \frac{32}{12}\lambda_i \int_\Omega Y_{O_{2_\Delta}}\phi_i\,dx + \lambda_i \int_\Omega Y_{O_{2_\Delta}}^2 \phi_i\,dx \\
&= \frac{32}{12}\lambda_i \int_\Omega \left[\eta_1\psi_0 + \sum_{j=1}^n y_j\psi_j\right]\phi_i\,dx + \lambda_i \int_\Omega \left[\eta_1\psi_0 + \sum_{j=1}^n y_j\psi_j\right]^2 \phi_i\,dx \\
&= \frac{32}{12}\lambda_i \int_\Omega \eta_1\psi_0\phi_i\,dx + \lambda_i \int_\Omega \eta_1^2\psi_0^2\phi_i\,dx + 2\lambda_i \int_\Omega \eta_1\psi_0 \sum_{j=1}^n y_j\psi_j\phi_i\,dx \\
&\quad + \frac{32}{12}\lambda_i \sum_{j=1}^n y_j \int_\Omega \psi_j\phi_i\,dx + \lambda_i \int_\Omega \left(\sum_{j=1}^n y_j\psi_j\right)^2 \phi_i\,dx \\
&:= \lambda_i\left[\frac{32}{12}J_i^a + J_i^b + 2J_i^c\right] + \frac{32}{12}\lambda_i J_i^d + \lambda_i J_i^e, \qquad i = 1,\dots,n
\end{aligned}$$

The next step is to take a closer look at the vectors $(J_i^{a,b,c})_{1\leq i\leq n}$ and rearrange them such that they can be added to the ODE system (3.3) as easily as possible. The main support during this endeavor will be the fact already used $supp\,(\psi_i \cdot \phi_j) = \emptyset \Leftrightarrow |i-j| \geq 2$, which holds true for hat functions.

$$a^r := \begin{pmatrix} 0 \\ J_1^a \\ J_2^a \\ \vdots \\ J_n^a \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1 \langle \psi_0, \phi_1 \rangle_{\mathscr{L}^2} \\ \eta_1 \langle \psi_0, \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \eta_1 \langle \psi_0, \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1 \frac{\Delta x}{6} \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} = \frac{\Delta x}{6} \begin{pmatrix} 0 \\ \eta_1 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

$$b^r := \begin{pmatrix} 0 \\ J_1^b \\ J_2^b \\ \vdots \\ J_n^b \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1^2 \langle \psi_0^2, \phi_1 \rangle_{\mathscr{L}^2} \\ \eta_1^2 \langle \psi_0^2, \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \eta_1^2 \langle \psi_0^2, \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1^2 \frac{\Delta x}{12} \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} = \frac{\Delta x}{12} \begin{pmatrix} 0 \\ \eta_1^2 \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

$$c^r := \begin{pmatrix} 0 \\ J_1^c \\ J_2^c \\ \vdots \\ J_n^c \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1 \langle \psi_0 \left(\sum_{j=1}^n y_j(t) \psi_j \right), \phi_1 \rangle_{\mathscr{L}^2} \\ \eta_1 \langle \psi_0 \left(\sum_{j=1}^n y_j(t) \psi_j \right), \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \eta_1 \langle \psi_0 \left(\sum_{j=1}^n y_j(t) \psi_j \right), \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_1 y_1(t) \langle \psi_0 \psi_1, \phi_1 \rangle_{\mathscr{L}^2} \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix} = \frac{\Delta x}{12} \begin{pmatrix} 0 \\ \eta_1 y_1(t) \\ 0 \\ \vdots \\ 0 \\ 0 \end{pmatrix}$$

Note that the calculation of b^r and c^r used the following values of the inner product:

$$r_{ij} := \langle \psi_j^2, \phi_i \rangle_{\mathscr{L}^2(\Omega)} = \int_0^1 \psi_j^2(x) \phi_i(x)\, dx \Rightarrow \; R^* := (r_{ij})_{1\leq i,j\leq n} = \Delta x \text{ tridiag} \left(\frac{1}{12}, \frac{1}{2}, \frac{1}{12} \right)$$

The vector $(J_i^d)_{1\leq i\leq n}$ can be expressed persuasively in terms of a matrix-vector notation with the same matrix M^* as in Section 3.1 as

$$\left(\sum_{j=1}^n y_j(t) \int_\Omega \psi_j \phi_i \, dx \right)_{1\leq i\leq n} = M^* y^*(t),$$

with the vector $y^*(t) := (y_i(t))_{1\leq i\leq n}$. In order to give a cohesive expression for the ODE system,

define the following matrix:

$$\overline{M} := \begin{pmatrix} 0 & \mathbf{0} & 0 \\ \mathbf{0} & M^* & \mathbf{0} \\ 0 & \mathbf{0} & 0 \end{pmatrix}$$

And, finally, examine the last vector with entries J_i^e. In this case, this is the most complicated one and that is the reason for primarily looking at the shape of one particular entry.

$$\begin{aligned} \int_\Omega \left(\sum_{j=1}^{n} y_j \psi_j \right)^2 \phi_i \, dx &= \int_\Omega \left(y_{i-1}\psi_{i-1} + y_i\psi_i + y_{i+1}\psi_{i+1} \right)^2 \phi_i \, dx \\ &= y_{i-1}^2 \langle \psi_{i-1}^2, \phi_i \rangle_{\mathscr{L}^2} + y_i^2 \langle \psi_i^2, \phi_i \rangle_{\mathscr{L}^2} + y_{i+1}^2 \langle \psi_{i+1}^2, \phi_i \rangle_{\mathscr{L}^2} \\ &+ 2y_{i-1}y_i \langle \psi_{i-1}\psi_i, \phi_i \rangle_{\mathscr{L}^2} + 2y_{i-1}y_{i+1} \langle \psi_{i-1}\psi_{i+1}, \phi_i \rangle_{\mathscr{L}^2} + 2y_i y_{i+1} \langle \psi_i \psi_{i+1}, \phi_i \rangle_{\mathscr{L}^2} \\ &= \frac{\Delta x}{12} \left[(y_{i-1} + y_i)^2 + 4y_i^2 + (y_{i+1} + y_i)^2 \right] \end{aligned}$$

With this calculation, we can assemble the last necessary vector that embodies the nonlinear character of the emerging system:

$$e^r := \begin{pmatrix} 0 \\ J_1^e \\ J_2^e \\ \vdots \\ J_{n-1}^e \\ J_n^e \\ 0 \end{pmatrix} = \frac{\Delta x}{12} \begin{pmatrix} 0 \\ (\eta_1 + y_1)^2 + 4y_1^2 + (y_2 + y_1)^2 \\ (y_1 + y_2)^2 + 4y_2^2 + (y_3 + y_2)^2 \\ \vdots \\ (y_{n-2} + y_{n-1})^2 + 4y_{n-1}^2 + (y_n + y_{n-1})^2 \\ (y_{n-1} + y_n)^2 + 4y_n^2 + (0 + y_n)^2 \\ 0 \end{pmatrix}$$

Altogether, with $\lambda := [\lambda_i]_{0 \le i \le n+1}$, the ODE system that emerges from PDE (4.1) and describes the mass fraction of the oxygen during the combustion is the following:

$$\boxed{\begin{aligned} M\frac{d}{dt}y(t) &= -\left[\nu C + D_g D\right] y(t) - \left[\nu b^c + D_g b^d\right] && \text{(4.5a)} \\ &\quad - \lambda \cdot \left[\frac{32}{12} a^r + b^r + 2c^r \right] - \frac{32}{12} \lambda \cdot \overline{M} y(t) - \lambda \cdot e^r && \text{(4.5b)} \\ y(0) &= \left[\exp^2(-1.5x_i) - x_i^{20} \exp^2(-1.5) \right]_{0 \le i \le n+1} && \text{(4.5c)} \end{aligned}}$$

Note that for vectors $a, b \in \mathbb{R}^{n+2}$ in this case the operation $a \cdot b$ describes element-wise multiplication.

4.2.2 Density of Gas and Fuel

Beginning with equation (4.2), there is not much to say, since this is just an algebraic relation in dependence of Y_{O_2}. Hence, we do not have to discretize anything and are able to simply obtain this quantity by inserting the mass fraction of oxygen. On the contrary, the MOL has to be carried out for PDE (4.3), as previously explained. In this case, we want to understand the complete right hand side of (4.3a) as the reaction term, i.e. $\mathcal{R}(\rho_F) = \rho_G Y_{O_2} A \exp\left(-\frac{E}{RT_F}\right)$. Note that, with this advance, the reaction term does not depend on ρ_F. In order to shorten notation, define again $\lambda_i := A \exp\left(-\frac{E}{RT_{F,i}}\right)$. Now, the discretization is the following:

$$\int_\Omega \mathcal{R}(\rho_{F_\Delta})\phi_i \, dx = \int_\Omega \rho_{G,i} Y_{O_2,i} \lambda_i \phi_i \, dx = \rho_{G,i} Y_{O_2,i} \lambda_i \int_\Omega \phi_i \, dx, \qquad i = 1, \ldots, n$$

We therefore get $\int_\Omega \phi_i \, dx = \Delta x$ for all $i = 1, \cdots, n$, and hence the complete discretized right hand side, supplemented with zero for the boundary points, can be constructed as

$$f^r(t) := \begin{pmatrix} 0 \\ \rho_{G,1}(t) Y_{O_2,1}(t) \lambda_1(t) \Delta x \\ \vdots \\ \rho_{G,n}(t) Y_{O_2,n}(t) \lambda_n(t) \Delta x \\ 0 \end{pmatrix}$$

and with that, the whole ODE system reads as follows:

$$\boxed{M \frac{d}{dt} y(t) = -f^r} \tag{4.6a}$$

$$\boxed{y(0) = \left[100\sqrt{x_i} + 10(1 - x_i)\right]_{0 \le i \le n+1}} \tag{4.6b}$$

At this juncture, we have to pay attention to the fact that the modeling wants to stop the reaction locally wherever $\rho_F < 10$. Assuming that, for an arbitrary instant of time $t_0 \in [0, T]$ and an inner spatial point x_k with $k \in \{1, \cdots, n\}$, $\rho_F(x_k, t_0) < 10$ holds true for the first time, then the demand for the pre-exponential factor is $A = 0$ and hence for the change in the density of the fuel, it shall hold $\frac{d}{dt} y_k(t) = 0$ wherever $t > t_0$. In order to give a note on programming this subtlety, the shape of the mass matrix M is inconvenient. Actually, a diagonal matrix would be very helpful for this purpose since in this case, it would be reasonable to simply set $f_k^r(t) = 0$ for $t \in (t_0, T]$ and directly obtain the requested yield. Fortunately, with our made choices of ansatz and test functions, the mass matrix M is regular, i.e. M^{-1} exists[9] and hence

[9] Additionally to simply use the inverse mass matrix, there is the possibility to use so-called *mass lumping* that transforms M into a diagonal matrix by defining the i^{th} diagonal element as the sum of the i^{th} row

we can equivalently consider the problem

$$\begin{aligned} Id_{n+2}\frac{d}{dt}y(t) &= -M^{-1}f^r \\ y(0) &= \left[100\sqrt{x_i} + 10(1-x_i)\right]_{0\le i\le n+1}, \end{aligned}$$

whereas Id_{n+2} delineates the (n+2)-dimensional identity matrix.

4.2.3 Temperature of Fuel

The aim in this section is to conduct the MOL for the PDE (4.4). Ultimately, we are facing a situation similar to the model PDE (2.4) with $\nu = 0$, $\delta = D_s$ and a slightly lenghty reaction term $-\mathcal{R}(T_F) = \frac{S_V\alpha}{\rho_F C_s^p}\left[T_G - T_F(x,t)\right] + \frac{\rho_G Y_{O_2}}{\rho_F C_s^p} A \exp\left(-\frac{E}{RT_F(x,t)}\right) LCV \cdot f$ by multiplying by -1. Again, the next step is to use the now well-known approximation procedure and to handle this reaction term. To contrive that, use the abbreviations $\vartheta_i := \frac{S_V\alpha}{\rho_{F,i}C_s^p}$ and $\xi_i := \frac{\rho_{G,i}Y_{O_2,i}}{\rho_{F,i}C_s^p} A \cdot LCV \cdot f$.

$$\begin{aligned} -\int_\Omega \mathcal{R}(T_{F_\Delta})\phi_i\,dx &= \vartheta_i \int_\Omega T_G\phi_i\,dx - \vartheta_i\int_\Omega T_{F_\Delta}\phi_i\,dx + \xi_i\int_\Omega \exp\left(-\frac{E}{RT_{F_\Delta}}\right)\phi_i\,dx \\ &= \vartheta_i T_G\int_\Omega \phi_i\,dx - \vartheta_i\int_\Omega\left[\eta_3\psi_0 + \sum_{j=1}^n y_j\psi_j + \beta_3\psi_{n+1}\right]\phi_i\,dx \\ &\quad + \xi_i\int_\Omega \exp\left(-\frac{E}{R}\left[\eta_3\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta_3\psi_{n+1}\right]^{-1}\right)\phi_i\,dx \\ &= \vartheta_i T_G\int_\Omega \phi_i\,dx - \vartheta_i\int_\Omega\left[\eta_3\psi_0 + \beta_3\psi_{n+1}\right]\phi_i\,dx - \vartheta_i\left(\sum_{j=1}^n y_j\right)\int_\Omega \psi_j\phi_i\,dx \\ &\quad + \xi_i\int_\Omega \exp\left(-\frac{E}{R}\left[\eta_3\psi_0 + \sum_{j=1}^n y_j(t)\psi_j + \beta_3\psi_{n+1}\right]^{-1}\right)\phi_i\,dx \\ &=: \vartheta_i K_i^g - \vartheta_i K_i^h - \vartheta_i K_i^l + \xi_i K_i^m, \qquad i = 1,\dots,n \end{aligned}$$

For better lucidity, let us analyze the above terms step by step.

$$g^r(t) := \begin{pmatrix} 0 \\ K_1^g \\ \vdots \\ K_n^g \\ 0 \end{pmatrix} = T_G \begin{pmatrix} 0 \\ \Delta x \\ \vdots \\ \Delta x \\ 0 \end{pmatrix}, \qquad l^r(t) := \begin{pmatrix} 0 \\ K_1^l \\ \vdots \\ K_n^l \\ 0 \end{pmatrix} = \overline{M}y(t)$$

and set the remaining elements to zero. This procedure is, for example, described in [GR07, pp.327-330].

$$h^r(t) := \begin{pmatrix} 0 \\ K_1^h \\ \vdots \\ K_n^h \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \langle \eta_3\psi_0 + \beta_3\psi_{n+1}, \phi_1 \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \eta_3\psi_0 + \beta_3\psi_{n+1}, \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \eta_3\langle \psi_0, \phi_1 \rangle_{\mathscr{L}^2} \\ \mathbf{0} \\ \beta_3\langle \psi_{n+1}, \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix} = \frac{\Delta x}{6} \begin{pmatrix} 0 \\ \eta_3 \\ \mathbf{0} \\ \beta_3 \\ 0 \end{pmatrix}$$

Note that the last computation again used $supp\,(\psi_i \cdot \phi_j) = \emptyset \Leftrightarrow |i-j| \geq 2$ to get the various zero elements. For the last term, cf. Section 3.2.2 because the vector C^r is very similiar to the following. Hence, we just have to adjust the previous case to the present one.

$$m^r := \begin{pmatrix} 0 \\ K_1^m \\ K_2^m \\ \vdots \\ K_{n-1}^m \\ K_n^m \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ \langle \exp\left(-\frac{E}{R}\left[\eta_3\psi_0 + y_1\psi_1 + y_2\psi_2\right]^{-1}\right), \phi_1 \rangle_{\mathscr{L}^2} \\ \langle \exp\left(-\frac{E}{R}\left[y_1\psi_1 + y_2\psi_2 + y_3\psi_3\right]^{-1}\right), \phi_2 \rangle_{\mathscr{L}^2} \\ \vdots \\ \langle \exp\left(-\frac{E}{R}\left[y_{n-1}\psi_{n-2} + y_{n-1}\psi_{n-1} + y_n\psi_n\right]^{-1}\right), \phi_{n-1} \rangle_{\mathscr{L}^2} \\ \langle \exp\left(-\frac{E}{R}\left[y_{n-1}\psi_{n-1} + y_n\psi_n + \beta_3\psi_{n+1}\right]^{-1}\right), \phi_n \rangle_{\mathscr{L}^2} \\ 0 \end{pmatrix}$$

Actually, like in the case of the convection diffusion reaction equation, it is not convenient to obtain a more compact expression for m^r analytically, but rather, a numerical integration for the occuring integrals is suggestive. Adding these vectors to the ODE-system with $\vartheta := [\vartheta_i]_{0\leq i\leq n+1}$, $\xi := [\xi_i]_{0\leq i\leq n+1}$ and again element-wise multiplication, the problem (4.4) reads as follows:

$$\boxed{M\frac{d}{dt}y(t) = -D_sDy(t) - D_sb^d + \vartheta \cdot [g^r - h^r - l^r] + \xi \cdot m^r} \tag{4.7a}$$

$$\boxed{y(0) = [500]_{0\leq i\leq n+1}} \tag{4.7b}$$

4.2.4 Outcome and Visualization

All in all, the ODE systems (4.5), (4.6) and (4.7) have to be solved simultaneously. Actually, it is slightly unpleasant to mark down the whole system and hence the abbreviations $RHSY_{O_2}$, $RHS\rho_F$ and $RHST_F$ shall be utilized for the vectors on the right hand side of the particular initial value problems. So the complete system that represents the MOL for the model equations

considered reads as follows:

$$\begin{pmatrix} M & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & M & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & M \end{pmatrix} \begin{pmatrix} \frac{d}{dt}Y_{O_{2,0}}(t) \\ \vdots \\ \frac{d}{dt}Y_{O_{2,n+1}}(t) \\ \frac{d}{dt}\rho_{F,0}(t) \\ \vdots \\ \frac{d}{dt}\rho_{F,n+1}(t) \\ \frac{d}{dt}T_{F,0}(t) \\ \vdots \\ \frac{d}{dt}T_{F,n+1}(t) \end{pmatrix} = \begin{pmatrix} RHSY_{O_{2,0}}(t) \\ \vdots \\ RHSY_{O_{2,n+1}}(t) \\ RHS\rho_{F,0}(t) \\ \vdots \\ RHS\rho_{F,n+1}(t) \\ RHST_{F,0}(t) \\ \vdots \\ RHST_{F,n+1}(t) \end{pmatrix} \tag{4.8}$$

Finally, a solution for this combustion model shall be presented with the following exemplary parameters: $\nu = 1.5$, $D_g = 1$, $A = 10$, $E = 7 \cdot 10^3$, $R = 8.315$, $p = 10^5$, $C_s^p = 1400$, $D_s = 0.005$, $S_V = 100$,$\alpha = 10$, $f = 0.3$ and $LCV = 32 \cdot 10^6$. Exactly as in Section 3.2, the programming took place in MATLAB and used *trapz* for the numerical integration of the functions of hat functions and *ODE15s* for solving the ODE system (4.8).

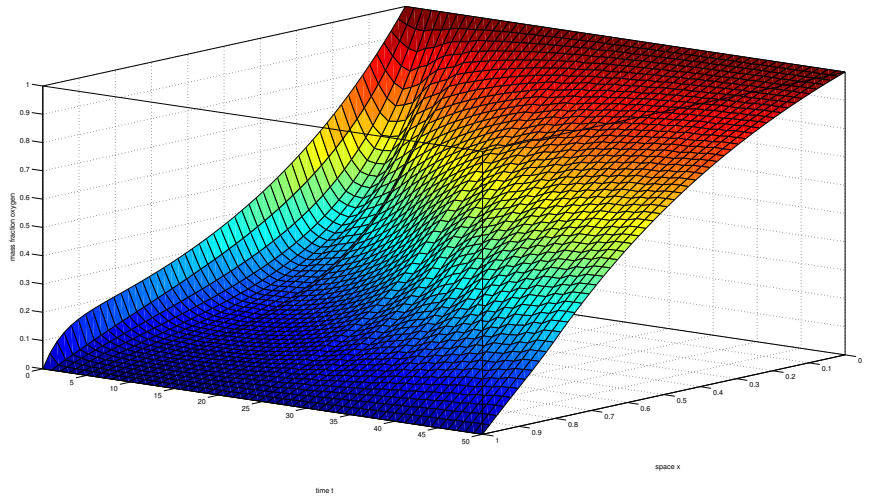


Figure 4.1: Mass Fraction of Oxygen with $T = 50$ and $n = 50$.

Note that the angle of view is different in each figure due to the relative best manner of observing the development. In the following, the results of the implementation will be discussed briefly. The mass fraction of the oxygen depicted in Figure (4.1) shows the meaningful decreasing behavior that is to be expected. One can see that the combustion requires oxygen in order to incinerate the carbon and, after terminating this procedure, Y_{O_2} tends to a steady state that averages between the stipulated conditions at the boudaries of Ω. Moreover, the density of the

gaseous mixture described by equation (4.2) shows exactly the opposite way around in Figure 4.2. This demeanor is caused by the fact that ρ_G is computed with Y_{O_2} in the denominator.

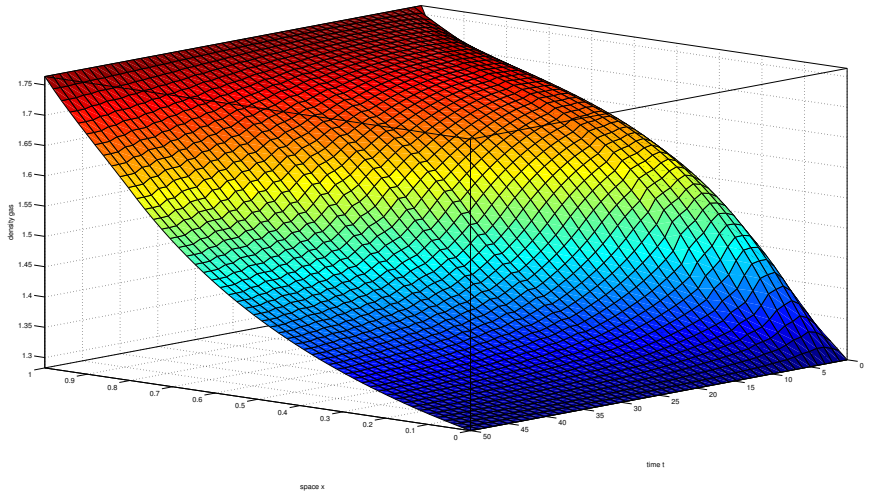


Figure 4.2: Density of the Gaseous Mixture with $T = 50$ and $n = 50$.

Figure 4.3 reveals the characteristics of the density of the fuel during the reaction. The density ρ_F abates slowly until the default value of (in this case) $10\frac{kg}{m^3}$ is attained and the fuel is entirely combusted. Regarding this, one can see where the so-called *reaction front*, i.e. the precise location of the combustion, is located both in time and space.

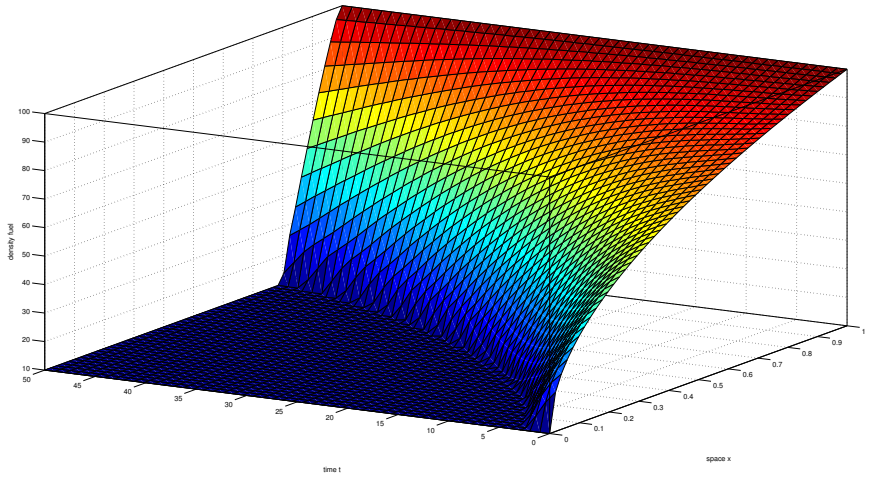


Figure 4.3: Density of the Fuel with $T = 50$ and $n = 50$.

The last quantity T_F is visualized in Figure 4.4 and shows the expedient growth of temperature. Furthermore, the leverage of the second spatial derivative is quite apparent, since, in an environment of the maximum temperature, the diffusion causes a dispersion of the temperature in all directions. Note that T_F declines gradually after attaining the ellipsoidal center of

combustion. In addition, the rise of temperature does not reach the upper boundary of Ω, as the timeframe regarded is not large enough.

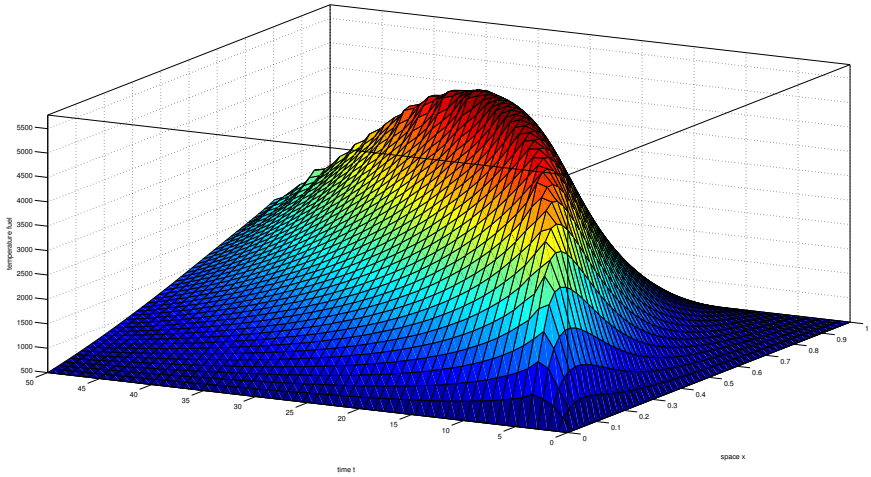
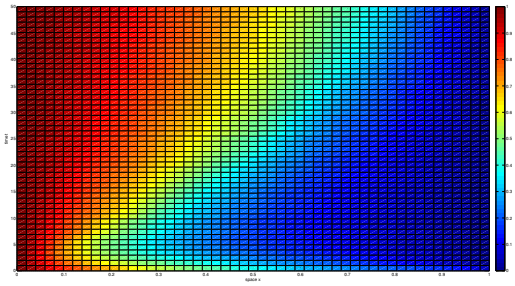
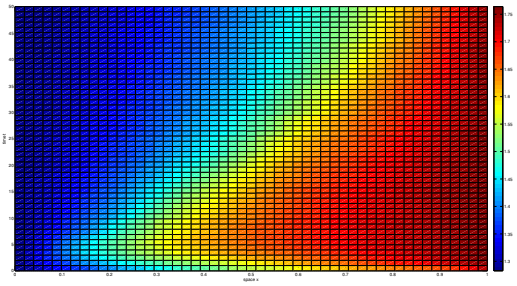


Figure 4.4: Temperature of the Fuel with $T = 50$ and $n = 50$.

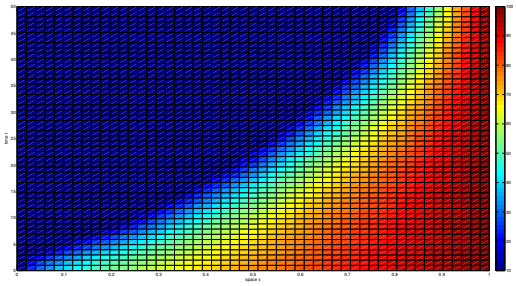
Finally, Figure 4.5 is a high-angle shot of all quantities that especially emphasizes the location of the reaction front and admits a different view than previous illustrations.



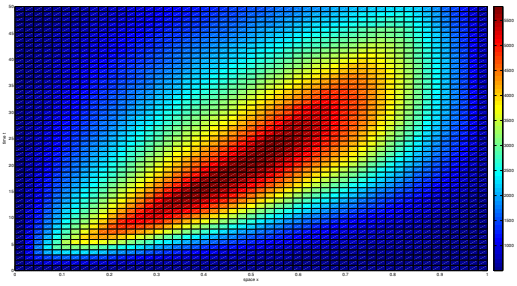
(a) Mass Fraction of Oxygen



(b) Density of Gaseous Mixture



(c) Density of Fuel



(d) Temperature of Fuel

Figure 4.5: Plan View on all Quantities.

CHAPTER 5

Summary and Future Prospects

This thesis characterized a potentiality to solve parabolic partial differential equations numerically by means of a finite element approach that converts the underlying equation into a semidiscrete one that can be solved by various methods for ordinary differential equations. Emphasis was placed on the treatment of occuring nonlinear source and sink terms that lead to nonlinear discretized equations and frequently required the employment of numerical integration procedures. The introduced model of combustion was solved, implemented in MATLAB and visualized using the previously obtained theoretical and numerical techniques.

A possibility to perpetuate this thesis would be to discuss the time discretization in more detail, i.e. for example, to describe Euler methods, Runge-Kutte methods, Adams-Moulton methods or backward differentiation formulas, which demand a great deal of attention because the Galerkin procedure yields systems of initial value problems that are usually stiff, requiring peculiar considerations in order to avoid disproportionate step sizes while preserving stability. It is certainly not coercive to use single-step or linear multistep methods exclusively. The so-called Discontinuous Galerkin method is a popular way to discretize the semidiscrete problem in time and is based upon a classical Galerkin approach with the arbitrative difference that the test function space used consists of piecewise discontinuous functions. Considering the Galerkin procedure, it is also feasible to use other functions than piecewise linear ones for the ansatz spaces in the spatial discretization. For example, piecewise quadratic functions, or in order to obtain even continuous differentiable basis functions, Hermite polynomials would als be reasonable. To give the last possible enhancement, so-called nonconforming finite element methods can also be advantageous. This modification alters the space V_Δ, in which a solution for the semidiscrete variational formulation is sought. Whereas the conforming methods explained in this thesis seek for a solution in a finite dimensional space that is contained in the space V belonging to the original variational formulation, noncomforming methods result from the situation $V_\Delta \nsubseteq V$.

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