

A Discontinuous Galerkin Method for Diffusion Flames

Embedded in a low-Mach solver framework

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Vorgelegte Dissertation von Juan Francisco Gutiérrez Jorquera aus Santiago, Chile

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Darmstadt, 8. November 2022

J. Gutiérrez-Jorquera



Abstract

Abstract



Zusammenfassung

Zusammenfassung



Acknowledgements

Mate + Faso + Merkelwave

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List of Abbreviations

\mathbf{u}_{ext} Extension-velocity field

List of Symbols

Ω	Domain of interest, computational domain
$\partial\Omega$	Domain boundary
\mathfrak{A}	Bulk phase A
\mathfrak{B}	Bulk phase B
s	Bulk phase, species
$\Omega \setminus \mathfrak{I}$	Bulk
\mathfrak{I}	Interface
\mathbf{w}	Singular surface velocity vector
w	Normal component of the singular surface velocity
$\mathbf{u}_{\mathfrak{I}}$	Material interface velocity vector
$\mathbf{n}_{\partial\Omega}$	Outer boundary normal vector
$\mathbf{n}_{\mathfrak{I}}$	Interface normal vector
\mathbf{n}	Normal vector
τ	Tangent vector
$\mathbf{P}_{\mathfrak{I}}$	Interface projection tensor
\mathbf{P}	Projection tensor
\mathbf{u}	Velocity vector
p	Pressure
e_{kin}	Kinetic energy
e_{σ}	Surface energy
ψ	General field/physical property
\mathbf{f}	Flux vector
μ	Dynamic viscosity
ν	Kinematic viscosity
σ	Surface tension coefficient
κ	Mean curvature
\mathbf{D}	Rate of deformation tensor
\mathbf{S}	Stress tensor
θ	Apparent contact angle
θ_{stat}	Static contact angle
L	Contact line
l_{cap}	Capillary length
l_s	Slip length
\mathbf{n}_L	Contact line normal vector
U_L	Contact line velocity
β	Coefficient of friction
c_p	Specific heat capacity of the mixture

$c_{p,k}$	Specific heat capacity of species k
T	Temperature
T_{sat}	Saturation temperature
\mathbf{q}	Heat flux vector
c	Specific heat capacity
k	Thermal conductivity
ρ	Density
\dot{m}	Mass transfer rate
h_{vap}	Enthalpy/(latent) heat of vaporization
D	Diffusion coefficient
ν_k	Stoichiometric coefficient of species k
A	Aggregation map
Agg	Aggregation mesh
N_k	Number of local DOF
N	Number of total DOF
\mathbf{Op}	Operator matrix
k	Total degree of the polynomial space
α	Aggregation threshold
ϕ	Basis function
\mathbb{P}_k	Broken polynomial space
K	Numerical cell
$K^{\mathbf{X}}$	Numerical cut-cell
\mathbf{X}	Cut
Δt	Time step size
Γ_D	Edge imposed with Dirichlet boundary condition
Γ_{int}	Internal edge
Γ_N	Edge imposed with Neumann boundary condition
Γ	Edge
h	Numerical mesh size
\mathfrak{K}_{cc}	Set of cut-cells
$\mathfrak{K}_{\text{far}}$	Set of far-field cells
$\mathfrak{K}_{\text{near}}$	Set of cut-cell neighbours
$\mathfrak{K}_h^{\mathbf{X}}$	Numerical cut-cell mesh
\mathfrak{K}_h	Numerical mesh
φ	Level-set function
Edg	Logical edge
\mathbf{M}	Mass matrix
\mathbf{n}_{Γ}	Edge normal field
$\mathbf{n}_{\mathfrak{I},\Gamma}$	Edge normal field including the interface normal vector
\hat{F}	Numerical flux
φ^{dg}	Level-set function represented by a DG field
φ^{co}	Constrained level-set function represented by a DG field
η	Penalty parameter
$\mathbb{V}_k^{\mathbf{X}}$	Sum of broken polynomial spaces
ϑ	General test function

q	Test function for the continuity equation
r	Test function for the heat equation
v	Test function for the momentum equation
ER	Expansion ratio the backward-facing step
Eo	tvös number
La	Laplace number
Pe	Peclet number
Fr	Froude number
ω	Oscillation frequency
λ	Wavelength
k	Wavenumber
g	Gravity vector
h	Channel heighth of the backward-facing step
\hat{h}	Convective heat transfer coefficient
λ	Heat conductivity
h_k	Specific enthalpy of k species.
Y_k	Mass fraction of species k
W	Mean molecular weight of the mixture
W_k	Molecular weight of species k
N	Total number of species in the mixture
Nu	Nusselt number
Nu_{loc}	Nusselt number, local
ω_k	Net rate of production of species k
Pr	Prandtl number
p	Pressure
\mathcal{R}	Universal gas constant
Re	Reynolds number
S	Step heighth of the backward-facing step
τ	Viscous tensor
t	Time
u	Velocity vector
D	Diffusion coefficient
U	Diffusion velocity vector

1 Introduction

1.1 Introduction and state of the art.

1.1.1 Combustion

Premixed Flames(???)

Non-Premixed Flames

Droplet(?)

High order discretization methods is a topic which has been gaining increasing attention in the last decades. An important exponent of them is the Discontinuous Galerkin (DG) method Cockburn et al., 2000. The DG method was initially developed and utilized for solving hyperbolic conservation laws, especially in the field of computational fluid dynamics (CFD), and has recently gained increased attention for incompressible CFD problems for structured and unstructured grids. Two main advantages stand out when compared with traditional methods such as the Finite Volume Method (FVM) or the Finite Difference Method (FDM): First, DG offers an arbitrary order of error convergence due to the polynomial local approximation of the solution field. A polynomial approximation of degree p provides a numerical discretization error of the order $\mathcal{O}(h^{p+1})$ for sufficiently smooth solutions, where h is a characteristic grid length. Secondly, regardless of the desired order of accuracy, any given cell of the grid only requires information from its immediate neighbours, allowing for efficient parallelization with minimal communication overhead. In contrast, more traditional schemes, such as the FVM, are usually limited to $\mathcal{O}(h^N)$ accuracy, with $N \leq 2$ for unstructured grids. Even for structured grids N is practically limited to low values due to the increasing stencil size for increasing N . Advantageously the DG method offers the locality of low-order schemes and the accuracy per degree of freedom of spectral schemes.

In the context of CFD solvers, an important distinction is that between pressure-based and density-based solvers. Historically, pressure-based solvers have been used for incompressible flows, i.e. flows with divergence-free velocity fields. On the other hand, density-based (also called fully compressible) solvers should, in theory, be able to solve flows in all Mach number ranges. However, in practice, as the Mach number approaches zero, density-based solvers experience efficiency and accuracy problems. These issues are mainly attributed to the acoustic effects in the flow, which tends to generate very stiff systems. None of these approaches are directly applicable to flows with varying density in the low-Mach limit. Hennink et al., 2021 It is possible, however, to extend existing incompressible and compressible codes so that they are capable of dealing with low Mach numbers. Keshtiban et al., 2003 In this work a extension from an incompressible solver is presented.

There are numerous works in which the DG method has been used within the context of

incompressible flows. Shahbazi et al., 2007; Kummer, 2012; Klein et al., 2013; Rhebergen et al., 2013 However, there are not many publications in which the flow problem at low Mach numbers is addressed using a pressure-based solver. In the work by Klein et al. Klein et al., 2016 the low-Mach equations are solved in a DG Framework making use of a SIMPLE type scheme. The solution of a time-step involves an iterative process that requires multiple matrix assemblies and solutions. The obtained systems of equations are solved by means of fixed-point iterations, where relaxation factors are necessary to obtain convergence of the computations. In the work of Hennink et al. Hennink et al., 2021 a pressure-based solver for low-mach flows is presented. They solve the mass flux instead of the velocity as the primitive variable.

High order methods are very attractive for complex reacting fluid dynamical systems, where usually a high numerical resolution is necessary. Particularly for combustion problems, where large amounts of heat are released in rather small zones within the flow, the high number of elements required to resolve the resulting steep gradients could result in prohibitive calculation times even for simple problems. In particular the study of so-called diffusion flames – also known as non-premixed flames – requires special consideration. In a diffusion flame, the reactants are initially spatially separated. For this kind of system, mixing plays a crucial role because reactants need to be brought together to the flame zone in order to maintain combustion. Many practical applications of diffusion flames consider deflagration flames, Poinsot and Veynante, 2005 which are characterized by a small characteristic velocity compared to the speed of sound. The low-Mach approximation of the Navier–Stokes equations is often chosen for describing this kind of system. This approximation allows for the calculation of non-constant density flows (such as temperature dependent density), while neglecting acoustic effects, thus dramatically reducing the required temporal resolution. Müller, 1998

In addition to the compressibility effects mentioned above, the need to accurately and efficiently represent the chemical reactions governing the combustion problem poses a major challenge. Generally speaking, to study the combustion process a detailed chemistry description is preferable. However, this is often impractical as it can be very intensive computationally speaking. Stauch et al. investigated systems with detailed mechanism for methanol combustion, where 23 chemical species and 166 elementary reactions are involved, Stauch et al., 2006 and for n-heptane with 62 chemical species and 572 elementary reactions, and with detailed transport processes Stauch and Maas, 2007. Because of their high complexity the mentioned works are restricted to simple one- or two-dimensional configurations, and to a small number of grid elements. If one is interested in more complex geometries or more complicated flow systems, the use of detailed kinetics can be prohibitive. Simplified kinetic models have been developed to overcome this difficulty. In the work of Westbrook et al. Westbrook and Dryer, 1981 a one-step kinetic model is presented, where combustion is expressed as a single chemical reaction with a reaction rate given by an Arrhenius-type expression with constant parameters. Multi-step chemical reaction models have also been developed, such as the four-step mechanism for methane combustion by Peters, Peters, 1985 or the three-step mechanism by Peters and Williams. Peters and Williams, 1987 Furthermore, extensions of one-step models exist, such as the one presented by Fernandez-Tarrazo et al. Fernandez-tarrazo et al., 2006 for hydrocarbon combustion with air, where kinetic parameters are correlated to the equivalence ratio in order to better describe characteristic flame properties for premixed and non-premixed flames.

In the last decades several numerical investigations related to diffusion flames have been carried out. Burke and Schumann were the first ones to investigate the structure of diffusion flames by studying the flame jet problem. Burke and Schumann, 1928 By assuming an infinitely fast chemical reaction they managed to predict flame properties fairly accurately. In the work of

Smooke et al. Smooke et al., 1986 a numerical simulation for a two-dimensional axisymmetric laminar diffusion jet with detailed chemistry was conducted and solved with Newton-type methods. In order to obtain adequate initial estimates for this problem, the solution of the problem for an infinitely fast chemistry was solved first. This idea was used in several works such as that by Keyes and Smooke Keyes and Smooke, 1987 for a counter diffusion flame, by Smooke Smooke and Giovangigli, 1992 for a Tsuji-counterflow configuration and in the work by Dobbins et al. Dobbins and Smooke, 2010 for an axisymmetric laminar jet diffusion flame with time dependent boundary conditions. In the work of Paxion Paxion et al., 2001 unstructured multigrid solver for laminar flames with detailed chemistry is presented. A Krylov-Newton method was used for solving several flame configurations. A two-dimensional counter diffusion flame was calculated, and its results were compared with the one-dimensional self-similar solution of the equations.

The DG method has also been used for simulations of combustion, mainly within a fully compressible framework. In the work from Johnson et al. Johnson and Kercher, 2020 the compressible Navier-Stokes equations are solved using a nodal DG scheme for combustion with complex chemistry and transport parameters. An hp-adaptive method is also presented, and shown to be useful for solving the ordinary differential equations used for describing the unsteady behaviour of the system. Similarly in the work from Lv and Ihme Lv and Ihme, 2017 a DG solver for multi-component chemically reacting flows, which solves the fully compressible Navier-Stokes equation, is presented. A hybrid-flux formulation is used, where a conservative Riemann solver is used for shock treatment, and a double-flux formulation is used in smooth regions. They show its applicability for non-reacting and reacting flows, particularly for systems characterized by high Mach numbers. On the other hand, the solution of combustion problems using the DG method in an incompressible framework is a topic that has not received much attention in the literature. This fact is the motivation of the present paper.

The system of equations obtained from the discretization of highly nonlinear systems can be very difficult to solve. Fixed-point iteration schemes have been used as a linearization strategy, as done by Klein et al. Klein et al., 2016 A major drawback of this approach is the highly problem dependent choice of under-relaxation factors. A much more robust strategy is the use of Newton type methods. Shadid et al., 1997; Pawlowski et al., 2006 Here, a problem-dependent factor is not needed. There is however a trade-off, because the Jacobian matrix has to be calculated, which can be computationally expensive. This approach has been used for combustion problems in numerous works. Karaa et al. Karaa et al., 2003 studied the axisymmetric laminar jet diffusion flame and investigated the behaviour of a multi-grid solver when using different pre-conditioners with a damped Newton algorithm. Shen et al. Shen et al., 2006 investigated the use and efficiency of a Newton method coupled with the Bi-CGSTAB method for an axisymmetric laminar jet flame. They concluded that, in terms of computational cost, the steady-state solution is more efficiently obtained by directly solving the steady formulation of the equations, than by solving the transient Navier-Stokes equations until the steady state is reached.

It is well known that the Newton method shows the property of having quadratic convergence sufficiently close to the solution Deuflhard, 2011. However, if the initial solution guess is not adequate, the method converge to a solution slowly, or may not even converge at all. For some highly nonlinear problems this is a significant issue. The so-called globalized Newton methods are used to overcome this problem by effectively increasing the area of convergence of the method. A popular globalized Newton method is the Newton-Dogleg method, Pawlowski et al., 2008 which is based on a trust-region technique.

In the present work, a steady low-Mach pressure-based solver for the simulation of temperature dependent non-reactive and reactive flows using the Discontinuous Galerkin method is presented. To the best of our knowledge, this is the first time that a pressure-based solver is used together with the DG method for solving the reactive low-Mach equations using the Newton-Dogleg method in a fully coupled manner. We focus in this study on two-dimensional configurations, but the ideas presented could be extended to three-dimensional systems. The one-step combustion model presented by Fernandez-Tarrazo et al. Fernandez-tarrazo et al., 2006 is used for describing the chemical reactions. In the present work we consider only methane combustion, but the one-step model could be used for other hydrocarbons as well. We choose this chemical model to obtain physically correct results for a wide range of applications, while avoiding the use of complex chemistry models. The discrete system of equations is solved by a globalized Newton method, by means of the Dogleg approach. In addition to the Newton-Dogleg method, a homotopy strategy is presented, which was found to be useful for obtaining solutions of steady state calculations of highly nonlinear problems. In order to find appropriate initial values for Newton's method in combustion applications, the concept of flame sheet estimates (i.e. the solution for infinitely fast chemistry) is used. Several benchmark cases are presented that allow us to validate our implementation. First we solve the differentially heated cavity problem, with which we intend to validate our implementation of the low-Mach solver for non-constant density flows using the fully coupled solver. Later two flame configurations are calculated, namely the counter-diffusion flame and the chambered diffusion flame. (Matalon et al., 1980)

In the following, we consider a two-dimensional system. However, the methods shown in this work could be also used for three-dimensional problems.

They were first derived by Rehm and Baum (Rehm and Baum, 1978). A rigorous extension to combustion problems was done by Majda and Sethian (Majda and Sethian, 1985).

2 Governing equations

In this work we present the methodology used to simulate reactive fluids in the low-Mach regime using the DG method. In this chapter we intend to show the governing equations, which will be discretized in the following chapters. First, in Section 2.1 the equations for a flow in the low-Mach regime with finite reaction velocity are shown. A brief derivation of the set low-Mach equations is presented, which should also serve as a way of showing and justifying the assumptions made in this work. We restricted ourselves to a one-step chemical model, but the algorithm presented could also be used for more complex chemistry models. Subsequently, in Section 2.2 the governing equations are shown for the case of assuming an irreversible chemical model with an infinite reaction rate. This case is often called the Burke–Schumann limit. These equations are used as part of the algorithm to solve the finite reaction rate case.

2.1 The low-Mach number equations for reactive flows

Combustion processes can be modeled by a system of nonlinear partial differential equations, namely the balance equations for total mass, momentum, energy, and mass of individual species (usually expressed in terms of mass fractions). This system needs to be solved together with an equation of state and expressions for the transport properties as well as for the chemical reaction rates. The derivation of the governing equations for a reacting flow system can be found in the literature. (see, for example, (Kee et al., 2003), (Poinsot and Veynante, 2005)). In the following pages, the main ideas regarding the derivation of equations are presented. For a more detailed explanation, we refer to the cited works and the references therein.

2.1.1 The reactive Navier–Stokes equations

Throughout this work, variables with a hat sign, e.g. $\hat{\rho}$ represent dimensional variables, while those without it are nondimensional. We start the derivation of the low-Mach number equations with the Navier–Stokes equations, the energy equation (in its temperature form), and the species transport equations. Let us consider a reacting fluid mixture composed of N species. Let $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z})$ and \hat{t} be the spatial vector and time. The primitive variables are the velocity field $\hat{\mathbf{u}} = (\hat{u}, \hat{v}, \hat{w})$, the pressure \hat{p} , the temperature \hat{T} , and the mass fractions Y_k of the N total

species. The set of governing equations to be solved is

$$\frac{\partial \hat{\rho}}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \hat{\mathbf{u}}) = 0, \quad (2.1a)$$

$$\frac{\partial \hat{\rho} \hat{\mathbf{u}}}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \hat{\mathbf{u}} \otimes \hat{\mathbf{u}}) = -\hat{\nabla} \hat{p} - \hat{\nabla} \cdot \hat{\tau} - \hat{\rho} \hat{\mathbf{g}}, \quad (2.1b)$$

$$\hat{\rho} \hat{c}_p \frac{\partial \hat{T}}{\partial \hat{t}} + \hat{\rho} \hat{c}_p \hat{\mathbf{u}} \cdot \hat{\nabla} \hat{T} = \frac{D\hat{p}}{Dt} - \hat{\nabla} \cdot \hat{\mathbf{q}} + \hat{\tau} : \hat{\nabla} \hat{\mathbf{u}} + \hat{\omega}_T \quad (2.1c)$$

$$\frac{\partial \hat{\rho} Y_k}{\partial \hat{t}} + \hat{\nabla} \cdot (\hat{\rho} \hat{\mathbf{u}} Y_k) = -\hat{\nabla} \cdot \hat{\mathbf{j}}_k + \hat{\omega}_k \quad (k = 1, \dots, N) \quad (2.1d)$$

This results in (in the general case) $N + 5$ differential equations to be solved. In these equations, $\hat{\rho}$ is the density of the mixture and $\hat{\mathbf{g}}$ is the acceleration of gravity. $\hat{\tau}$, $\hat{\mathbf{q}}$ and $\hat{\mathbf{j}}_k$ are the viscous tensor, the heat flux vector and the molecular mass flux vector of species k , respectively. Additionally, $\hat{\omega}_T$ is the heat release due to combustion and $\hat{\omega}_k$ is the reaction rate of species k . To close the system, expressions must be defined to link these variables with the primitive variables. They will be briefly shown and commented upon in the following paragraphs.

Equation of state

Assuming that the fluid behaves ideally, the density can be calculated as

$$\hat{\rho} = \frac{\hat{p} \hat{W}_{avg}}{\mathcal{R} \hat{T}}. \quad (2.2)$$

Here, $\hat{\mathcal{R}}$ is the universal gas constant of gases, and \hat{W}_{avg} is the average molecular weight of the fluid, defined as

$$\hat{W}_{avg} = \left(\sum_{k=1}^N \frac{Y_k}{\hat{W}_k} \right)^{-1} \quad (2.3)$$

with \hat{W}_k as the molecular weight of species k . For an ideal mixture, the specific heat capacity can be calculated as weighted averages of the specific heats of the species,

$$\hat{c}_p = \sum_{k=1}^N Y_k \hat{c}_{p,k}, \quad (2.4)$$

where $\hat{c}_{p,k}$ corresponds to the specific heat capacity of the component k . The temperature dependence of $\hat{c}_{p,k}$ can be accounted for by using NASA polynomials (Mcbride et al., 1993).

$$\hat{c}_{p,k} = \left(\hat{a}_1 + \hat{a}_2 \hat{T} + \hat{a}_3 \hat{T}^2 + \hat{a}_4 \hat{T}^3 + \hat{a}_5 \hat{T}^4 \right) \frac{\hat{\mathcal{R}}}{\hat{W}_k} \quad (2.5)$$

where $\hat{a}_1, \hat{a}_2, \hat{a}_3, \hat{a}_4$ and \hat{a}_5 are numerical coefficients supplied by the NASA database.

Transport models

The viscous tensor $\hat{\tau}$ is defined for a Newtonian fluid as

$$\hat{\tau} = -\hat{\mu} \left(\hat{\nabla} \hat{\mathbf{u}} + (\hat{\nabla} \hat{\mathbf{u}})^T \right) + \left(\frac{2}{3} \hat{\mu} - \hat{\kappa} \right) (\hat{\nabla} \cdot \hat{\mathbf{u}}) \mathbf{I} \quad (2.6)$$

Here, $\hat{\mu}$ is the dynamic viscosity of the fluid, which is generally specific to the fluids and depends on its temperature and pressure. Furthermore, $\hat{\kappa}$ corresponds to the bulk viscosity, which is usually negligible for fluids at low pressures (Bird et al., 1960). $\hat{\kappa}$ will be taken equal to zero in the rest of this work.

The heat flux vector $\hat{\mathbf{q}}$ is given by Fourier's law of heat conduction,

$$\hat{\mathbf{q}} = \hat{\lambda} \hat{\nabla} \hat{T}. \quad (2.7)$$

Here $\hat{\lambda}$ corresponds to thermal conductivity, which, similar to the viscosity, is dependent on the particular fluid under study and its temperature and pressure.

The molecular mass flux vector $\hat{\mathbf{j}}_k$ of species k is defined as $\hat{\mathbf{j}}_k = \hat{\rho} \hat{\mathbf{U}}_k$. Here $\hat{\mathbf{U}}_k$ is the diffusion velocity of the component k . In general, $\hat{\mathbf{U}}_k$ can be obtained by solving the Maxwell-Stefan equations.

$$\nabla X_p = \sum_{k=1}^N \frac{X_p X_k}{D_{pk}} (\mathbf{U}_k - \mathbf{U}_p) \quad p = 1, \dots, N. \quad (2.8)$$

Here $D_{pk} = D_{kp}$ is the binary mass diffusion coefficient of species p in species k . X_p is the mole fraction of species k and is related to the mass fraction of k as $X_k = Y_k \hat{W}/\hat{W}_k$. The solution of the system (2.8) is often a difficult and costly task (Williams, 2000; Poinsot and Veynante, 2005), and often simplifications are made. It can be shown that for binary mixtures ($N = 2$) and for mixtures containing multiple species ($N > 2$) where all diffusion coefficients are equal, the system (2.8) reduces exactly to the well-known Fick's law.

$$\hat{\mathbf{j}}_k = -\hat{\rho} \hat{D}_k \nabla Y_k \quad (2.9)$$

This expression is only exact in the cases mentioned above. For a system where the heat capacities of each species are different, this expression is inconsistent. The variable \hat{D}_k corresponds in this case to the diffusion coefficient of species k in the mixture. An issue regarding the global mass conservation can be pointed out here. Recall that by definition the sum of the mass fractions must always be one ($\sum_k^N Y_k = 1$). This is only true for the solution of Equation (2.1) if exact expressions for the diffusion velocities are used (Poinsot and Veynante, 2005). If some inexact expression is used (as for example Fick's law), the constraint for the sum of the mass fractions will not be fulfilled. This problem can be surpassed by solving the global mass conservation (continuity) equation Equation (2.1a) and only the equations for the first $N - 1$ species Equation (2.1d). Therefore, all inconsistencies that originated from not using an exact species diffusion model are absorbed by Y_N . As pointed out in Poinsot and Veynante, 2005, this simplification should only be used if all $N - 1$ species are strongly diluted in species N , such as the case of a flame in air, where the mass fraction of nitrogen is large. It can also be noted that this approach reduces in one the number of differential equations needed to be solved.

The temperature dependence of viscosity can be modeled by Sutherland's law (Sutherland, 1893)

$$\hat{\mu}(\hat{T}) = \hat{\mu}_{\text{suth}} \left(\frac{\hat{T}}{\hat{T}_{\text{suth}}} \right)^{1.5} \frac{\hat{T}_{\text{suth}} + \hat{S}}{\hat{T} + \hat{S}}. \quad (2.10)$$

Here $\hat{\mu}_{\text{suth}}$ is the viscosity evaluated at a reference temperature \hat{T}_{suth} , and \hat{S} is a material dependent parameter. In all calculations in this work the value of \hat{S} for air is used, $\hat{S} = 110.5$ K. Expressions for determining the thermal conductivity and diffusion coefficients as function of temperature can be obtained using similar expressions, as will be shown later in Section 2.1.2

Chemical model

Consider a system composed of N species where M chemical reactions take place. Chemical reactions can be written in generalized form as follows.

$$\sum_{k=1}^N \nu'_{kj} \mathcal{M}_k \rightleftharpoons \sum_{k=1}^N \nu''_{kj} \mathcal{M}_k \quad \text{for } j = 1, \dots, M \quad (2.11)$$

where ν'_{jk} and ν''_{jk} are the molar stoichiometric coefficients of species k in the chemical reaction j , and \mathcal{M}_j represents the chemical component k .

The reaction rate of species k is $\hat{\omega}_k$, which accounts for the total amount of species k that appear or disappear due to M chemical reactions (c.f. Equations (2.11)). Its given by

$$\hat{\omega}_k = \hat{W}_k \sum_{j=1}^M \nu_{jk} \hat{\mathcal{Q}}_j. \quad (2.12)$$

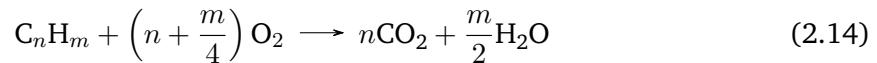
Here $\nu_{kj} = \nu''_{kj} - \nu'_{kj}$, and \mathcal{Q}_j is the rate of progress of the reaction j . They are usually modeled using Arrhenius-type expressions, as will be shown later.

The heat release $\hat{\omega}_T$ that appears in the energy equation is related to the reaction rates according to

$$\hat{\omega}_T = - \sum_{k=1}^N \hat{h}_k \hat{\omega}_k = - \sum_{k=1}^N \Delta \hat{h}_k^0 \hat{\omega}_k - \sum_{k=1}^N \hat{h}_{ks} \hat{\omega}_k \quad (2.13)$$

Here, the specific enthalpy of k -th species \hat{h}_k is written in terms of its formation enthalpy \hat{h}_k^0 and a sensible enthalpy $\hat{h}_{ks} = \int_0^{\hat{T}} \hat{c}_{p,k} d\hat{T}$. The second term on the right-hand side of Equation (2.13) is usually small and is exactly zero for a mixture where all the heat capacities of each component are equal (Poinsot and Veynante, 2005). It will be neglected in the rest of the analysis.

In this work, we use the one-step kinetic model for the combustion of hydrocarbons presented in Fernandez-tarrazo et al., 2006. The chemical reaction is represented by a single ($M = 1$) exothermic global irreversible expression as



The rate of progress of the global reaction is modeled by an Arrhenius-type expression

$$\hat{\mathcal{Q}} = \hat{B} e^{-\hat{T}_a/\hat{T}} \left(\frac{\hat{\rho} Y_F}{\hat{W}_F} \right)^a \left(\frac{\hat{\rho} Y_O}{\hat{W}_O} \right)^b. \quad (2.15)$$

Here, the subscripts F and O refer to fuel and oxidizer, respectively. The parameter \hat{B} corresponds to the pre-exponential factor, \hat{T}_a is the activation temperature, and a and b are reaction orders. For a one-step reaction model, the reaction rate of the k -th component (Equation (2.12)) is

$$\hat{\omega}_k = \nu_k \hat{W}_k \hat{\mathcal{Q}}. \quad (2.16)$$

\hat{B} (cm ³ /(mol s))	\hat{T}_{a0} (K)	\hat{Q}_0 (MJ kmol ⁻¹)	a	b
6.9×10^{14}	15 900	802.4	1	1

Table 2.1: Base parameters used in the one-step combustion model by Fernandez-tarrazo et al., 2006

With this definition, the heat release $\hat{\omega}_T$ (Equation (2.13)) is

$$\hat{\omega}_T = -\hat{W}_F \hat{\omega}_F \hat{Q}^m = -\hat{\omega}_F \hat{Q}. \quad (2.17)$$

Here is \hat{Q}^m the molar heat of reaction of the one-step reaction and \hat{Q} is the mass heat of reaction. \hat{W}_F and $\hat{\omega}_F$ are the molar mass of the fuel species and the reaction rate of the fuel species respectively.

Within the model from (Fernandez-tarrazo et al., 2006), several parameters are adjusted to represent characteristic features of premixed flames and diffusion flames. The parameters \hat{T}_a and \hat{Q} are defined as functions of the local equivalence ratio ϕ , which is, in turn, defined in terms of the local mass fractions of fuel Y_F and oxidizer Y_O as

$$\phi = \frac{s Y_F^0}{Y_O^0} \frac{s Y_F - Y_O + Y_O^0}{s(Y_F^0 - Y_F) + Y_O}, \quad (2.18)$$

where Y_F^0 and Y_O^0 are the mass fractions of the fuel and oxidizer flows in their corresponding feed streams, and s is the mass stoichiometric ratio, defined as $s = \nu_O \hat{W}_O / \nu_F \hat{W}_F$. The activation energy and molar heat release depend on ϕ as

$$\hat{T}_a(\phi) = \begin{cases} (1 + 8.250(\phi - 0.64)^2) \hat{T}_{a0} & \text{if } \phi \leq 0.64, \\ \hat{T}_{a0} & \text{if } 0.64 \leq \phi \leq 1.07, \\ (1 + 4.443(\phi - 1.07)^2) \hat{T}_{a0} & \text{if } \phi \geq 1.07, \end{cases} \quad (2.19)$$

$$\hat{Q}(\phi) = \begin{cases} \hat{Q}_0 & \text{if } \phi \leq 1 \\ (1 - \alpha(\phi - 1)) \hat{Q}_0 & \text{if } \phi > 1, \end{cases} \quad (2.20)$$

The parameter α is a constant that depends on the hydrocarbon being considered. In particular $\alpha = 0.21$ for the combustion of methane.

2.1.2 The unsteady non-dimensional low-Mach equations

In the present work, we use the low-Mach number equation approximation of the governing equations. The derivation of the equations can be found in (**mullerLowMachNumberAsymptoticsNavierStokes** Rehm and Baum, 1978; Majda and Sethian, 1985). We refer to these references for a detailed explanation on how the set of equations is derived. In the following, we restrict ourselves to show and comment on the main consequences of the low-Mach limit.

The low-Mach number limit approximation of the governing equations is used for flows where the Mach number (defined as $\text{Ma} = \hat{u}_{\text{ref}}/\hat{c}$, where \hat{u}_{ref} is a characteristic flow velocity and \hat{c} the speed of sound) is small, which is usually the case in typical laminar combustion systems. (Dobbins and Smooke, 2010). The low-Mach equations are obtained by using standard

asymptotic methods. One of the main results of the analysis is that for flows with a small Mach number, the pressure can be decomposed as

$$\hat{p}(\hat{\mathbf{x}}, \hat{t}) = \hat{p}_0(\hat{t}) + \hat{p}_2(\hat{\mathbf{x}}, \hat{t}). \quad (2.21)$$

The spatially uniform term $\hat{p}_0(\hat{t})$ is called thermodynamic pressure, and only appears in the equation of state. It is constant in space, but can change in time. For an open system, the thermodynamic pressure is constant and equal to the ambient pressure, while for a closed system (e.g. a system completely bounded by walls) it changes in order to ensure mass conservation. On the other hand, the perturbational term $\hat{p}_2(\hat{\mathbf{x}}, \hat{t})$ appears only in the momentum equations and plays a role similar to that of the pressure in the classical incompressible formulation. This perturbational term satisfies $\hat{p}_2/\hat{p} \sim \mathcal{O}(\text{Ma})^2$, (Dobbins and Smooke, 2010; Nonaka et al., 2018) showing that under these assumptions, the equation of state is satisfied only to $\mathcal{O}(\text{Ma}^2)$ (cf. Equation (2.2))

Effectively, the low-Mach limit of the Navier-Stokes equations allows for the calculation of systems where big density variations due to temperature differences are present, thus not restricting ourselves to approximations such as the Boussinesq approximation for buoyancy-driven flow. In addition, this approximation truncates the mechanism of pressure wave propagation which is a natural feature of the compressible Navier-Stokes equations. In doing this, we are no longer restricted to choosing small timesteps to be able to resolve wave phenomena, and the maximum allowed timestep is greatly increased. From now on we will drop the sub-index of the hydrodynamic pressure \hat{p}_2 and we will refer to it simply as \hat{p} , further emphasizing the similarity in its role to the pressure of the incompressible formula.

In this work we use a non-dimensional formulation of the governing equations. We define the non-dimensional quantities.

$$\begin{aligned} \rho &= \frac{\hat{\rho}}{\hat{\rho}_{\text{ref}}}, & p &= \frac{\hat{p}}{\hat{p}_{\text{ref}}}, & \mathbf{u} &= \frac{\hat{\mathbf{u}}}{\hat{u}_{\text{ref}}}, & T &= \frac{\hat{T}}{\hat{T}_{\text{ref}}}, & c_p &= \frac{\hat{c}_p}{\hat{c}_{p,\text{ref}}}, & W_k &= \frac{\hat{W}_k}{\hat{W}_{\text{ref}}} \\ \mu &= \frac{\hat{\mu}}{\hat{\mu}_{\text{ref}}}, & D_k &= \frac{\hat{D}_k}{\hat{D}_{k,\text{ref}}}, & k &= \frac{\hat{k}}{\hat{k}_{\text{ref}}}, & \nabla &= \frac{\hat{\nabla}}{\hat{L}_{\text{ref}}}, & t &= \frac{\hat{t}}{\hat{t}_{\text{ref}}}, & \mathbf{g} &= \frac{\hat{\mathbf{g}}}{\hat{g}_{\text{ref}}}, & Q &= \frac{\hat{Q}}{\hat{Q}_0} \end{aligned}$$

Here \hat{u}_{ref} , \hat{L}_{ref} , \hat{p}_{ref} , \hat{t}_{ref} , and \hat{T}_{ref} are the reference velocity, length, pressure, time, and temperature, respectively, and are equal to some characteristic value for the particular configuration studied. Furthermore, \hat{g}_{ref} is the magnitude of the gravitational acceleration and \hat{W}_{ref} is the reference molecular weight. The reference transport properties $\hat{\mu}_{\text{ref}}$, \hat{k}_{ref} , $\hat{D}_{k,\text{ref}}$ and the reference heat capacity of the mixture and $\hat{c}_{p,\text{ref}}$ are evaluated at the reference temperature \hat{T}_{ref} . Similarly, the reference density must satisfy the equation of state, thus $\hat{\rho}_{\text{ref}} = \hat{p}_{\text{ref}} / (\hat{R} \hat{T}_{\text{ref}} \hat{W}_{\text{ref}})$. By introducing these definitions into the governing equations (Equations (2.1a) to (2.1d)) the reactive set of non-dimensional low-Mach number equations is obtained. The system of differential equations to be solved reads as follows.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (2.22a)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) - \frac{1}{\text{Fr}^2} \rho \mathbf{g}, \quad (2.22b)$$

$$\frac{\partial \rho T}{\partial t} + \nabla \cdot (\rho \mathbf{u} T) = \frac{1}{\text{Re} \text{Pr}} \nabla \cdot \left(\frac{k}{c_p} \nabla T \right) + \text{H Da} \frac{Q \mathcal{Q}}{c_p}, \quad (2.22c)$$

$$\frac{\partial \rho Y_k}{\partial t} + \nabla \cdot (\rho \mathbf{u} Y_k) = \frac{1}{\text{Re} \text{Pr} \text{Le}_k} \nabla \cdot (\rho D \nabla Y_k) + \text{Da} \nu_k W_k \mathcal{Q}. \quad (k = 1, \dots, N-1) \quad (2.22d)$$

Note that we assumed that the spatial gradients of the mixture heat capacity are small, allowing us to introduce it in the derivative of the diffusive term of Equation (2.22c). Furthermore, using the fact that the sum of the mass fractions must always be one, the mass fraction of the last species N can be calculated with

$$Y_N = 1 - \sum_{k=1}^{N-1} Y_k. \quad (2.23)$$

The N -th component mass fraction Y_N is calculated using Equation (2.23). This system is solved for the primitive variables velocity $\mathbf{u} = (u_x, u_y)$, pressure p , temperature T and mass fractions $\mathbf{Y} = (Y_1, \dots, Y_N)$. We note that the form of the low-Mach equations is very similar to the Navier-Stokes equations. The greatest difference is in the decomposition of the pressure, as mentioned above. This similarity is beneficial, as it allows the use of similar techniques to solve the PDE system to those used for the completely incompressible case (Keshtiban et al., 2003).

Six non-dimensional factors arise from the non-dimensionalization process:

$$\begin{aligned} \text{Re} &= \frac{\hat{\rho}_{\text{ref}} \hat{u}_{\text{ref}} \hat{L}_{\text{ref}}}{\hat{\mu}_{\text{ref}}}, & \text{Fr} &= \frac{\hat{u}_{\text{ref}}}{\sqrt{\hat{g}_{\text{ref}} \hat{L}_{\text{ref}}}}, & \text{Pr} &= \frac{\hat{c}_{p,\text{ref}} \hat{\mu}_{\text{ref}}}{\hat{k}_{\text{ref}}}, \\ \text{Le}_k &= \frac{\hat{k}_{\text{ref}}}{\hat{\rho}_{\text{ref}} \hat{D}_{k,\text{ref}} \hat{c}_{p,\text{ref}}}, & \text{Da} &= \frac{\hat{B} \hat{L}_{\text{ref}} \hat{\rho}_{\text{ref}}}{\hat{M}_{\text{ref}} \hat{u}_{\text{ref}}}, & \text{H} &= \frac{\hat{Q}_0}{\hat{c}_{p,\text{ref}} \hat{T}_{\text{ref}}} \end{aligned}$$

The first three equations define the Reynolds, Froude and Prandtl number respectively. Le_k is the Lewis number of species k . Finally Da and H are the Damköhler number and the non-dimensional heat release respectively. The non-dimensional progress of the global reaction reads as follows.

$$\mathcal{Q}(T, \mathbf{Y}) = \left(\frac{\rho Y_F}{M_F} \right) \left(\frac{\rho Y_O}{M_O} \right) \exp \left(\frac{-T_a}{T} \right), \quad (2.24)$$

where $T_a = \hat{T}_a / \hat{T}_{\text{ref}}$. Furthermore, the non-dimensional heat release is

$$Q(\phi) = \begin{cases} 1 & \text{if } \phi \leq 1 \\ (1 - \alpha(\phi - 1)) & \text{if } \phi > 1, \end{cases} \quad (2.25)$$

with ϕ evaluated according to Equation (2.18). In the low-Mach limit, the ideal gas equation depends on the thermodynamic pressure, temperature and mass fractions. It reads in its non-dimensional form

$$\rho(p_0, T, \mathbf{Y}) = \frac{p_0}{T \sum_{k=1}^N \frac{Y_k}{W_k}}. \quad (2.26)$$

As mentioned above, the thermodynamic pressure of a closed system is a parameter that has to be determined (for an open system is equal to the atmospheric pressure). Defining the initial mass of the fluid inside the closed system as m_0 , and by integrating Equation (2.26) on the whole domain Ω , one obtains

$$p_0(T, \mathbf{Y}) = \frac{m_0}{\int_{\Omega} \frac{W_{\text{avg}}}{T} dV}, \quad (2.27)$$

TODO: porque tengo escrito aca la cosa con Wavg??? Similarly, the non-dimensional specific heat capacity of the mixture c_p is calculated as

$$c_p(T, \mathbf{Y}) = \sum_{k=1}^N Y_k c_{p,\alpha}(T), \quad (2.28)$$

and the non-dimensional viscosity as

$$\mu(T) = T^{\frac{3}{2}} \frac{1 + \hat{S}}{\hat{T}_{\text{ref}} T + \hat{S}}. \quad (2.29)$$

As mentioned before, the model for the transport parameters can be simplified by assuming constant values for the Prandtl and Lewis numbers. (Smoke and Giovangigli, 1991) and we can write $\mu(T) = k/c_p(T) = \rho D_k(T)$.

2.2 The flame sheet approximation

Here we introduce the concept of the flame sheet approximation, which is used in our solution algorithm for solving the finite reaction rate system given by Equations (2.1a), (2.1b), (2.22c) and (2.22d). We follow the ideas proposed in the work from Keyes and Smooke, 1987. Assuming that all species have the same constant heat capacity c_p and mass diffusion coefficient $D_k = D$, that the Lewis number is unity for all species, and that combustion can be described by a single-step chemical reaction, it is possible to obtain an equation for a scalar without source terms, taking a linear combination of the energy Equation (2.22c) and mass fraction Equation (2.22d). A commonly used scalar is the mixture fraction z , which per definition is equal to unity in the fuel feed stream, and equal to zero in the oxidizer feed stream. Thus, the system of Equations (2.1a), (2.1b), (2.22c) and (2.22d) can be simplified to solving the low-Mach Navier-Stokes equations together with an equation for the passive scalar z :

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0, \quad (2.30a)$$

$$\frac{\partial \rho \mathbf{u}}{\partial t} + \nabla \cdot (\rho \mathbf{u} \otimes \mathbf{u}) = -\nabla p + \frac{1}{\text{Re}} \nabla \cdot \mu \left(\nabla \mathbf{u} + \nabla \mathbf{u}^T - \frac{2}{3} (\nabla \cdot \mathbf{u}) \mathbf{I} \right) - \frac{1}{\text{Fr}^2} \rho \mathbf{g}, \quad (2.30b)$$

$$\frac{\partial \rho z}{\partial t} + \nabla \cdot (\rho \mathbf{u} z) = \frac{1}{\text{Re} \text{Pr}} \nabla \cdot (\rho D \nabla z), \quad (2.30c)$$

which are solved together with the equation of state and expressions for the transport parameters. Note that the system is not closed, because ρ , μ and ρD are still functions of temperature and mass fractions. These fields can be related to the mixture fraction using the concept of the Burke-Schumann flame structure. (Burke and Schumann, 1928) In the case of an infinitely fast chemical reaction, fuel and oxidizer cannot co-exist. On one side of this sheet only oxidizer is found, and on the other side only fuel. The exact position of the flame sheet can be determined by finding the location of points where both reactant mass fractions Y_F and Y_O meet in stoichiometric proportions, that is, the points where the mixture fraction $z = z_{st}$, with

$$z_{st} = \frac{Y_O^0}{Y_O^0 + s Y_F^0}, \quad (2.31)$$

where Y_O^0 is the mass fraction of oxidizer in the oxidizer inlet stream, and Y_F^0 is the mass fraction of fuel in the fuel inlet stream. The Burke-Schumann solution provides analytical expressions for temperature and mass fraction fields on either side of the flame sheet as function of the mixture fraction z (see for example the textbook from Poinsot and Veynante, 2005 or the work from Keyes and Smooke, 1987).

$$T(z) = \begin{cases} zT_F^0 + (1-z)T_O^0 + \frac{QY_F^0}{c_p}z_{st}\frac{1-z}{1-z_{st}} & \text{if } z \geq z_{st} \\ zT_F^0 + (1-z)T_O^0 + \frac{QY_F^0}{c_p}z & \text{if } z < z_{st} \end{cases} \quad (2.32)$$

The mass fraction field of fuel and oxidizer species at either side of the flame are given by:

$$Y_F(z) = \begin{cases} Y_F^0\frac{z - z_{st}}{1 - z_{st}} & \text{if } z \geq z_{st} \\ 0 & \text{if } z < z_{st} \end{cases} \quad (2.33)$$

$$Y_O(z) = \begin{cases} 0 & \text{if } z \geq z_{st} \\ Y_O^0\left(1 - \frac{z}{z_{st}}\right) & \text{if } z < z_{st} \end{cases} \quad (2.34)$$

and finally, the mass fraction field of product species P is:

$$Y_P(z) = \begin{cases} Y_O^0\frac{W_P\nu_P}{W_O\nu_O}(1-z) & \text{if } z \geq z_{st} \\ Y_F^0\frac{W_P\nu_P}{W_F\nu_F}z & \text{if } z < z_{st} \end{cases} \quad (2.35)$$

Once the mixture fraction field z is obtained, the temperature and mass fraction fields are uniquely defined by Equations (2.32) to (2.35), which are used to evaluate the density and the transport properties. This coupling between variables and the associated nonlinear system leads to the need for an iterative solution scheme.

The main idea of introducing this additional system (Equations (2.30a) to (2.30c)) is to find an approximate solution to the system where a finite reaction-rate is used (Equations (2.22a) to (2.22d)). In Figure 2.1 temperature and fuel mass fraction fields across the center-line of a counterflow flame configuration is shown. Clearly, both solutions are very similar, differing only in the area near the flame. However, this similarity is only valid under the assumptions made to derive Equation (2.30c). In the case that the Lewis number is not equal to one, or that the heat capacities are not equal for each species, the finite-rate solution will differ slightly from that obtained with the infinite-reaction rate.

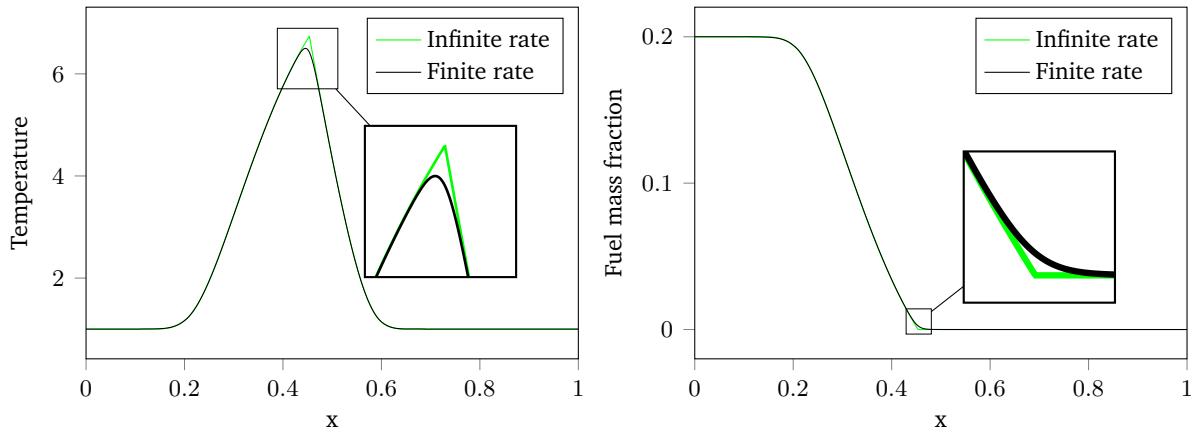


Figure 2.1: Temperature and fuel mass fraction profiles calculated in the center-line of a counter-flow flame configuration using finite chemistry (black) and the flame sheet approximation (green).

2.3 Boundary conditions

The following boundary conditions are imposed for the resolution of the finite reaction rate system (Equations (2.22a) to (2.22d)) and for the flame sheet problem (Equations (2.30a) to (2.30c)).

$$\Gamma_D : \mathbf{u} = \mathbf{u}_D, T = T_D, Y_k = Y_{k,D}, z = z_D, \quad (2.36a)$$

$$\Gamma_{DW} : \mathbf{u} = \mathbf{u}_D, \nabla T \cdot \mathbf{n}_{\partial\Omega} = 0, \nabla Y_k \cdot \mathbf{n}_{\partial\Omega} = 0, \nabla z \cdot \mathbf{n}_{\partial\Omega} = 0, \quad (2.36b)$$

$$\begin{aligned} \Gamma_N : & \left(-p\mathbf{I} + \left(\frac{\mu}{Re} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) \right) \cdot \mathbf{n}_{\partial\Omega} = 0, \\ & \nabla T \cdot \mathbf{n}_{\partial\Omega} = 0, \nabla Y_k \cdot \mathbf{n}_{\partial\Omega} = 0, \nabla z \cdot \mathbf{n}_{\partial\Omega} = 0, \end{aligned} \quad (2.36c)$$

$$\begin{aligned} \Gamma_{ND} : & \left(-p\mathbf{I} + \left(\frac{\mu}{Re} (\nabla \mathbf{u} + (\nabla \mathbf{u})^T) - \frac{2}{3}\mu(\nabla \cdot \mathbf{u})\mathbf{I} \right) \right) \cdot \mathbf{n}_{\partial\Omega} = 0, \\ & T = T_D, Y_k = Y_{k,D}, z = z_D \end{aligned} \quad (2.36d)$$

$$\Gamma_P : \mathbf{u}(\mathbf{x}) = \mathbf{u}(\mathbf{x}'), T(\mathbf{x}) = T(\mathbf{x}'), Y_k(\mathbf{x}) = Y_k(\mathbf{x}'), z(\mathbf{x}) = z(\mathbf{x}'), \quad (2.36e)$$

where k denotes the index from mass fractions $k = (1, \dots, N - 1)$. The boundary Γ_D represents conditions for inlets and walls, with velocity, temperature, mass fractions and mixture fraction defined as Dirichlet boundary conditions. Boundaries Γ_{DW} are used to represent adiabatic walls, where velocity is given as a Dirichlet boundary condition, but with the gradients perpendicular to the wall of the transported scalars set to zero. The boundary Γ_N represent an outflow of the domain with homogeneous Neumann condition for all scalars. The boundary Γ_{ND} also represents an outlet boundary condition, but with Dirichlet boundary conditions for the scalars. Finally the boundaries Γ_P are periodic boundaries, where \mathbf{x} and \mathbf{x}' are periodic pairs in the domain.

3 Numerical methods

3.1 The Discontinuous Galerkin method

3.1.1 Spatial discretization

We start by introducing some standard definitions and notation in the context of DG methods: Kummer, 2017 Kikker et al., 2020 We define a computational domain $\Omega \subset \mathbb{R}^2$ with a polygonal and simply connected boundary $\partial\Omega$. Our numerical grid is then defined by the set of non-overlapping elements $\mathcal{K} = \{K_1, \dots, K_N\}$ with a characteristic mesh size h , so that Ω is the union of all elements, i.e. $\Omega = \bigcup_{i=1}^N K_i$. We define $\Gamma = \bigcup_j \partial K_j$ as the union of all edges (internal edges and boundary edges) and $\Gamma_I = \Gamma \setminus \partial\Omega$ as the union of all interior edges. For each edge of Γ a normal field \mathbf{n}_Γ is defined. Particularly on $\partial\Omega$ is defined as an outer normal and $\mathbf{n}_\Gamma = \mathbf{n}_{\partial\Omega}$. For each field $\mathbf{u} \in C^0(\Omega \setminus \Gamma_I)$ we define \mathbf{u}^- and \mathbf{u}^+ , which describe the information in the interior and exterior sides of the cell:

$$\mathbf{u}^- = \lim_{\xi \searrow 0} \mathbf{u}(\mathbf{x} - \xi \mathbf{n}_\Gamma) \quad \text{for } \mathbf{x} \in \Gamma \quad (3.1)$$

$$\mathbf{u}^+ = \lim_{\xi \searrow 0} \mathbf{u}(\mathbf{x} + \xi \mathbf{n}_\Gamma) \quad \text{for } \mathbf{x} \in \Gamma_I \quad (3.2)$$

The jump and mean values of \mathbf{u} on inner edges Γ_I are defined as:

$$[\![\mathbf{u}]\!] = \mathbf{u}^+ - \mathbf{u}^- \quad (3.3)$$

$$\{\mathbf{u}\} = \frac{1}{2} (\mathbf{u}^- + \mathbf{u}^+) . \quad (3.4)$$

while the jump and mean values on boundary edges $\partial\Omega$ are:

$$[\![\mathbf{u}]\!] = \mathbf{u}^- \quad (3.5)$$

$$\{\mathbf{u}\} = \mathbf{u}^- . \quad (3.6)$$

We define the broken polynomial space of total degree k as

$$\mathbb{P}_k(\mathcal{K}_h) = \{f \in L^2(\Omega) ; \forall K \in \mathcal{K} : f|_K \text{ is polynomial and } \deg(f|_K) \leq k\}. \quad (3.7)$$

Additionally for $u \in C^1(\Omega \setminus \Gamma)$ the broken gradient $\nabla_h u$ is defined as:

$$\nabla_h u = \begin{cases} 0 & \text{on } \Gamma \\ \nabla u & \text{elsewhere} \end{cases} \quad (3.8)$$

The broken divergence $\nabla_h \cdot u$ is defined analogously. Finally, we define the function space for test and trial functions for D_v dependent variables:

$$\mathbb{V}_\mathbf{k} = \prod_{i=1}^{D_v} \mathbb{P}_{k_i}(K_h) \quad (3.9)$$

where $\mathbf{k} = (k_1, \dots, k_{D_v})$.

3.1.2 Discretization for a DG Method

As an introductory example, following **hesthaven_nodal_2008**, we are considering the discretization of a general conservation law with a non-linear flux function $\mathbf{f}(\psi)$ for a scalar quantity $\psi = \psi(\mathbf{x}, t)$ in Ω and suitable Dirichlet boundary condition on $\partial\Omega = \partial\Omega_D$ and a compatible initial condition ψ_0 . The problem statement reads

$$\frac{\partial\psi}{\partial t} + \nabla \cdot \mathbf{f}(\psi) = 0, \quad \mathbf{x} \in \Omega, \quad (3.10a)$$

$$\psi = \psi_D, \quad \mathbf{x} \in \partial\Omega_D, \quad (3.10b)$$

$$\psi(\mathbf{x}, 0) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \Omega. \quad (3.10c)$$

The goal is to find an approximate solution $\tilde{\psi} = \tilde{\psi}(\mathbf{x}, t)$ to ψ that fulfils the problem (3.10). Therefore, the problem domain Ω is discretized by a numerical mesh \mathfrak{K}_h and for each numerical cell K_j we introduce the approximation by a local polynomial basis $\phi_j = (\phi_{j,l})_{l=1,\dots,N_k} \in \mathbb{P}_k(\{K_j\})$ with a cell-local support $\text{supp}(\phi_j) = \bar{K}_j$ as

$$\psi_j(\mathbf{x}, t) = \sum_{l=1}^{N_k} \tilde{\psi}_{j,l}(t) \phi_{j,l}(\mathbf{x}) = \tilde{\psi}_j(t) \cdot \phi_j(\mathbf{x}), \quad \mathbf{x} \in K_j, \quad (3.11)$$

where the coefficients $\tilde{\psi}_j = (\tilde{\psi}_{j,l})_{l=1,\dots,N_k}$ denote the unknowns or degrees of freedom (DOF) of the local solution in cell K_j . In this work a modal polynomial basis is used, which fulfils the orthogonality condition

$$\int_{K_j} \phi_{j,m} \phi_{j,n} \, dV = \delta_{mn} \quad (3.12)$$

with the Kronecker delta δ_{mn} . Inserting the local approximation (3.11) into the conservation law (3.10a) results in a cell-wise residual

$$R_j(\mathbf{x}, t) = \frac{\partial\psi_j}{\partial t} + \nabla \cdot \mathbf{f}(\psi_j), \quad \mathbf{x} \in K_j. \quad (3.13)$$

For a Galerkin method, the residual (3.13) is minimized with respect to the same space as the ansatz functions, i.e. $\mathbb{P}_k(\{K_j\})$. Thus, we demand for the test functions $\vartheta_{j,l} = \phi_{j,l}$ in each cell $K_j \in \mathfrak{K}_h$ that

$$\int_{K_j} R_j \vartheta_{j,l} \, dV = \int_{K_j} \frac{\partial\psi_j}{\partial t} \phi_{j,l} + \nabla \cdot \mathbf{f}(\psi_j) \phi_{j,l} \, dV \stackrel{!}{=} 0, \quad \forall \phi_{j,l}. \quad (3.14)$$

So, for each cell we end up with a linear system of N_k equations. However so far, no approximate global solution $\psi \in \Omega$ can be regained from the minimization in (3.14). The global solution is assumed to be a piecewise polynomial approximation

$$\psi(\mathbf{x}, t) \approx \psi(\mathbf{x}, t) = \bigoplus_{j=1}^J \psi_j(\mathbf{x}, t) = \sum_{j=1}^J \sum_{l=1}^{N_k} \tilde{\psi}_{j,l}(t) \phi_{j,l}(\mathbf{x}) \in \mathbb{P}_k(\mathfrak{K}_h) \quad (3.15)$$

defined as the direct sum of the J local solutions ψ_j in (3.11). Here, $\tilde{\psi}_{j,l}$, with $j = 1, \dots, J$ and $l = 1, \dots, N_k$, denote the total DOF, with $N = J \cdot N_k$, of the global approximate solution ψ . In

order to formulate a global DG method, the spatial term on the right-hand side of equation (3.14) is rewritten in terms of boundary edge integrals $\forall K_j \in \mathcal{K}_h$ using partial integration

$$\int_{K_j} \frac{\partial \psi_j}{\partial t} \phi_{j,l} \, dV - \int_{K_j} \mathbf{f}(\psi_j) \cdot \nabla_h \phi_{j,l} \, dV + \oint_{\partial K_j} (\mathbf{f}(\psi_j) \cdot \mathbf{n}_j) \phi_{j,l} \, dS = 0, \quad \forall \phi_{j,l}, \quad (3.16)$$

where \mathbf{n}_j represents the local outward pointing normal for cell K_j . Note that on the internal edges Γ_{int} the value of $\mathbf{f}(\psi_j)$ is multiply defined. Therefore, a numerical flux \hat{F} is introduced

$$\hat{F}(\psi_j^{\text{in}}, \psi_j^{\text{out}}, \mathbf{n}_\Gamma) \approx \mathbf{f}(\psi_j) \cdot \mathbf{n}_j, \quad (3.17)$$

that uniquely defines the resulting value of both neighbouring values, i.e. ψ_j^{in} and ψ_j^{out} at internal edges Γ_{int} . Summing over all cells K_j , the global minimization problem for $\psi(\mathbf{x}, t), \mathbf{x} \in \Omega$ reads: Find $\psi \in \mathbb{P}_k(\mathcal{K}_h)$, such that $\forall \vartheta = \phi \in \mathbb{P}_k(\mathcal{K}_h)$

$$\int_{\Omega} \frac{\partial \psi}{\partial t} \phi \, dV - \int_{\Omega} \mathbf{f}(\psi) \cdot \nabla_h \phi \, dV + \oint_{\Gamma} \hat{F}(\psi^{\text{in}}, \psi^{\text{out}}, \mathbf{n}_\Gamma) [\phi] \, dS = 0, \quad (3.18)$$

where at Γ_D the outer value $\psi^{\text{out}} = \psi_D$ is given by the Dirichlet boundary condition (3.10b). In order to fully discretize the initial boundary value problem (3.10), one further needs to discretize the temporal term. This issue is skipped at this point and is discussed in Section ???. Thus, the current form of (3.18) is referred to as the semi-discrete weak formulation of (3.10).

Considering the spatial discretization, the numerical flux \hat{F} needs to satisfy certain mathematical and physical properties to ensure stability and convergence of the DG method. In this work the stability is defined in the continuous setting via the energy estimate

$$\|\psi(\mathbf{x}, t)\|_\Omega^2 \leq \|\psi(\mathbf{x}, 0)\|_\Omega^2, \quad \forall t \geq 0, \quad (3.19)$$

where homogenous Dirichlet conditions are assumed. Thus, stability is given, if the energy $\|\psi(\mathbf{x}, t)\|_\Omega^2$ only decreases in the absence of an inflow. Two properties need to be fulfilled in order to proof that the discrete problem (3.18) satisfies the discrete equivalent of the energy estimate in (3.19). The numerical flux \hat{F} is required to be a function that is Lipschitz continuous and monotonic, see [di_pietro_mathematical_2012](#) for the proof. Furthermore, it is obvious that the DG method needs to regain a unique approximate solution to the underlying problem. Thus, \hat{F} satisfies the following consistency property

$$\hat{F}(a, a, \mathbf{n}) = \mathbf{f}(a) \cdot \mathbf{n}, \quad \forall a \in \mathbb{R}. \quad (3.20)$$

A direct consequence of (3.20) is that the weak formulation (3.18) is directly fulfilled for $\psi = \psi$. Since considering a general conservation law in its conservative form, one further requires that \hat{F} regains the global conservation property, i.e. the total amount of ψ only changes due to fluxes across the domain boundary $\partial\Omega$, by satisfying

$$\hat{F}(a, b, \mathbf{n}) = -\hat{F}(a, b, -\mathbf{n}), \quad \forall a, b \in \mathbb{R}. \quad (3.21)$$

The specific form of a suitable numerical flux \hat{F} is presented in Section ??, where the spatial discretization of the two-phase flow problem is discussed.

Note that the system (3.18) can be written in a shorten matrix formulation as

$$\mathbf{M} \frac{d\tilde{\psi}}{dt} + \mathbf{Op}(\tilde{\psi}) = \mathbf{b}, \quad (3.22)$$

where the sought-after coefficients are given as the solution vector $\tilde{\psi} = \{\tilde{\psi}_{1,1}, \tilde{\psi}_{1,2}, \dots, \tilde{\psi}_{j,n}, \dots, \tilde{\psi}_{J,N_k}\} \in \mathbb{R}^N$. The mass matrix $\mathbf{M} \in \mathbb{R}^{N \times N}$ has a block-diagonal structure with

$$\mathbf{M} = \begin{bmatrix} \mathbf{M}_1 & 0 & \cdots & 0 \\ 0 & \mathbf{M}_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{M}_J \end{bmatrix}, \quad (3.23)$$

where the cell-local mass matrix \mathbf{M}_j is defined by

$$(\mathbf{M}_j)_{m,n} = \int_{K_j} \phi_{j,m} \phi_{j,n} \, dV = \int_{K_j} \phi_j \otimes \phi_j \, dV. \quad (3.24)$$

The cell-local Operator matrix \mathbf{Op}_j is given by

$$(\mathbf{Op}_j)_{m,n} = - \int_{K_j} \mathbf{f}(\tilde{\psi}_{j,n} \phi_{j,n}) \cdot \nabla_h \phi_{j,m} \, dV + \oint_{\partial K_j} \hat{F}(\tilde{\psi}_{j,n}, \tilde{\psi}_{j^*,n}, \mathbf{n}_j) \phi_{j,m} \, dS, \quad (3.25)$$

where j^* denotes the index of a neighbouring cell to K_j . Like the mass matrix, the operator matrix exhibits a block-diagonal structure, but including secondary diagonals due to the coupling with neighbouring cells over the numerical fluxes \hat{F} . The right-hand side \mathbf{b} incorporates the given Dirichlet boundary condition value ψ_D .

Discontinuous Galerkin discretization of the finite reaction rate problem

We start by presenting the DG discretization of the finite reaction system defined by ??–2.22d. We define $\mathbf{Y}' = (Y_1, \dots, Y_{N-1})$ as the vector containing the first $(n_s - 1)$ mass fractions and $\mathbf{s} = (s_1, \dots, s_{N-1})$ as the vector containing the test functions for the first $(n_s - 1)$ mass fraction equations. The discretized form of ???? and Equations (2.22c) and (2.22d) is obtained by multiplying each equation by a test function, integrating it over an element K , applying integration by parts and finally using an adequate numerical flux for each term. Note that the convective and diffusive terms of the temperature scalars T , mass fraction Y_α and mixture fraction z have the same form, so they share the same expression in their discretized form. In order to ensure the validity of the Ladyzenskaja-Babuška-Brezzi (or inf-sup) condition, Babuška, 1973 we use a mixed order formulation, where polynomials of order k for velocity, temperature and mass fractions, and of degree $k' = k - 1$ for pressure are used. Finally the discretized problem can be written as: find the numerical solution $(p_h, \mathbf{u}_h, T_h, \mathbf{Y}'_h) \in \mathbb{V}_k$ such that for all test functions $(q_h, \mathbf{v}_h, r_h, \mathbf{s}_h) \in \mathbb{V}_k$ we have:

$$\mathcal{B}^1(q_h) = \mathcal{C}(\mathbf{u}_h, q_h, \rho(T_h, \mathbf{Y}_h)) , , \quad (3.26a)$$

$$\begin{aligned} \mathcal{B}^2(\mathbf{v}_h) = & \mathcal{U}^C(\mathbf{u}_h, \mathbf{u}_h, \mathbf{v}_h, \rho(T_h, \mathbf{Y}_h)) + \mathcal{U}^P(p_h, \mathbf{v}_h) + \frac{1}{\text{Re}} \mathcal{U}^D(\mathbf{u}_h, \mathbf{v}_h, \mu(T_h)) \\ & + \frac{1}{\text{Fr}^2} \mathcal{U}^S(\rho(T_h, \mathbf{Y}_h), \mathbf{v}_h) , \end{aligned} \quad (3.26b)$$

$$\begin{aligned} \mathcal{B}^3(r_h) = & \mathcal{S}^C(\mathbf{u}_h, T_h, r_h, \rho(T_h, \mathbf{Y}_h)) + \frac{1}{\text{Re} \, \text{Pr}} \mathcal{S}^D(T_h, r_h, k/c_p(T_h)) \\ & + \text{H Da} \, \mathcal{S}^S(r_h, Q(T_h, \mathbf{Y}_h), \omega(T_h, \mathbf{Y}_h), c_p(T_h, \mathbf{Y}_h)) , \end{aligned} \quad (3.26c)$$

$$\begin{aligned} \mathcal{B}^3(s_{\alpha h}) = & \mathcal{S}^C(\mathbf{u}_h, Y_{\alpha h}, s_{\alpha h}, \rho(T_h, \mathbf{Y}_h)) + \frac{1}{\text{Re} \, \text{Pr} \, \text{Le}_\alpha} \mathcal{S}^D(Y_{\alpha h}, s_{\alpha h}, \rho D_\alpha(T_h)) \\ & + \text{Da} \mathcal{M}_\alpha^S(s_{\alpha h}, \omega(T_h, \mathbf{Y}_h)) . \end{aligned} \quad (3.26d)$$

where the index α takes values $\alpha = 1, \dots, (n_s - 1)$. The n_s -th component mass fraction Y_{n_s} is calculated using Equation (2.23).

Discontinuous Galerkin discretization of the flame sheet problem

Discretizing the flame sheet problem given by Equations (2.30a) to (2.30c) proceeds in a similar way. Due to the similarity of the mass fraction equation and the mixture fraction equation the discretization is analogous. Again, we use a mixed order formulation of polynomials of degree k for velocity and mixture fraction, and of degree $k - 1$ for pressure. The resulting problem reads: find the numerical solution $(p_h, \mathbf{u}_h, z_h) \in \mathbb{V}_k$ such that for all test functions $(q_h, \mathbf{v}_h, r_h) \in \mathbb{V}_k$ we have:

$$\mathcal{B}^1(q_h) = \mathcal{C}(\mathbf{u}_h, q_h, \rho(z_h)), \quad (3.27a)$$

$$\begin{aligned} \mathcal{B}^2(\mathbf{v}_h) &= \mathcal{U}^C(\mathbf{w}_h, \mathbf{u}_h, \mathbf{v}_h, \rho(z_h)) + \mathcal{U}^P(p_h, \mathbf{v}_h) + \frac{1}{\text{Re}} \mathcal{U}^D(\mathbf{u}_h, \mathbf{v}_h, \mu(z_h)) \\ &\quad + \frac{1}{\text{Fr}^2} \mathcal{U}^S(\rho(z), \mathbf{v}_h), \end{aligned} \quad (3.27b)$$

$$\mathcal{B}^3(r_h) = \mathcal{S}^C(\mathbf{u}_h, z_h, r_h, \rho(z_h)) + \frac{1}{\text{Re} \text{Pr}} \mathcal{S}^D(z_h, r_h, \rho D(z_h)). \quad (3.27c)$$

Note that density and transport parameters are dependent on the mixture fraction z . The evaluation of those parameters is done as mentioned in ?? and solved iteratively using a Newton-Dogleg type method as shown later in Section 3.2.1

Definitions of nonlinear forms

We show in the following the nonlinear forms used in this work. Regarding the choice of fluxes, we follow the "best practices" known in literature for the incompressible Navier-Stokes equation. It is known Pietro and Ern, 2012; Girault et al., 2004 that central difference fluxes for the pressure gradient and velocity divergence, combined with a coercive form for the viscous terms, e.g. symmetric interior penalty, gives a stable discretization for the Stokes equation. Furthermore, it is known that for all kinds of convective terms, a numerical flux which transports information in characteristic direction, e.g. Upwind, Lax-Friedrichs or Local-Lax-Friedrichs, must be used. We opted for the last one in our implementation, as it offers a good compromise between accuracy and stability.

Continuity equation We use a central difference flux for the discretization of the continuity equation:

$$\mathcal{C}(\mathbf{u}, q, \rho) = \oint_{\Gamma_l \cup \Gamma_N \cup \Gamma_{ND} \cup \Gamma_P} \{\rho \mathbf{u}\} \cdot \mathbf{n}_\Gamma \llbracket q \rrbracket \, dS - \int_\Omega \rho \mathbf{u} \cdot \nabla_h q \, dV. \quad (3.28)$$

The density in Equation (3.28) is evaluated as a function of the temperature and mass fractions using the equation of state (Equation (2.26)). The term \mathcal{B}^1 on the right hand sides of Equation (3.26a) and Equation (3.27a) contains the Dirichlet boundary conditions:

$$\mathcal{B}^1(q) = - \oint_{\Gamma_D \cup \Gamma_{DW}} q (\rho_D \mathbf{u}_D \cdot \mathbf{n}_\Gamma) \cdot dS \quad (3.29)$$

The density at the boundary ρ_D is evaluated with Equation (2.26) using the corresponding Dirichlet values of temperature and mass fractions.

Momentum equations The convective term of the momentum equations is discretized using a Lax-Friedrichs flux

$$\mathcal{U}^C(\mathbf{w}, \mathbf{u}, \mathbf{v}, \rho) = \oint_{\Gamma} \left(\{\rho \mathbf{u} \otimes \mathbf{w}\} \mathbf{n}_{\Gamma} + \frac{\gamma_1}{2} [\![\mathbf{u}]\!] \right) \cdot [\![\mathbf{v}]\!] \, dS - \int_{\Omega} (\rho \mathbf{u} \otimes \mathbf{w}) : \nabla_h \mathbf{v} \, dV. \quad (3.30)$$

The Lax-Friedrichs parameter γ_1 is calculated as Klein et al., 2016

$$\gamma_1 = \max \left\{ 2\overline{\rho^+} |\overline{\mathbf{u}^+} \cdot \mathbf{n}^+|, 2\overline{\rho^-} |\overline{\mathbf{u}^-} \cdot \mathbf{n}^-| \right\}, \quad (3.31)$$

where $\overline{\rho_h^{\pm}}$ and $\overline{\mathbf{u}^{\pm}}$ are the mean values of ρ^{\pm} and \mathbf{u}^{\pm} in K^{\pm} , respectively. The pressure term is discretized by using a central difference flux

$$\mathcal{U}^P(p, \mathbf{v}) = \oint_{\Gamma \setminus \Gamma_N \setminus \Gamma_{ND}} \{p\} ([\![\mathbf{v}]\!] \cdot \mathbf{n}) \, dS - \int_{\Omega} p \nabla_h \mathbf{v} \, dV. \quad (3.32)$$

The diffusive term of the momentum equations is discretized using an Symmetric Interior Penalty (SIP) formulation Shahbazi, 2005

$$\begin{aligned} \mathcal{U}^D(\mathbf{u}, \mathbf{v}, \mu) = & \int_{\Omega} \left(\mu \left((\nabla_h \mathbf{u}) + (\nabla_h \mathbf{u})^T - \frac{2}{3} (\nabla_h \cdot \mathbf{u}) \mathbf{I} \right) \right) : \nabla_h \mathbf{v} \, dV \\ & - \oint_{\Gamma \setminus \Gamma_N \setminus \Gamma_{ND}} \left(\left\{ \mu (\nabla_h \mathbf{u} + \nabla_h \mathbf{u}^T - \frac{2}{3} (\nabla_h \cdot \mathbf{u}) \mathbf{I}) \right\} \mathbf{n}_{\Gamma} \right) \cdot [\![\mathbf{v}]\!] \, dS \\ & - \oint_{\Gamma \setminus \Gamma_N \setminus \Gamma_{ND}} \left(\left\{ \mu (\nabla_h \mathbf{v} + \nabla_h \mathbf{v}^T - \frac{2}{3} (\nabla_h \cdot \mathbf{v}) \mathbf{I}) \right\} \mathbf{n}_{\Gamma} \right) \cdot [\![\mathbf{u}]\!] \, dS \\ & + \oint_{\Gamma \setminus \Gamma_N \setminus \Gamma_{ND}} \eta \mu_{max} [\![\mathbf{u}]\!] [\![\mathbf{v}]\!] \, dS. \end{aligned} \quad (3.33)$$

The viscosity μ is evaluated as a function of temperature according to Equation (2.29) and $\mu_{max} = \max(\mu^+, \mu^-)$. Additionally η is the penalty term of the SIP formulation, which has to be chosen big enough to ensure coercivity of the form, but also as small as possible in order to not increase the condition number of the problem. The estimation of the penalty term is based on an expression of the form

$$\eta = \eta_0 \frac{A(\partial K)}{V(K)}, \quad (3.34)$$

where for a two-dimensional problem A is the perimeter and V the area of the element. Parameter η_0 is a safety factor. If not stated otherwise, the value $\eta_0 = 4$ is set in all calculations. Further information on the determination of the penalty term can be found in [hillewaertDevelopmentDiscontinuousGalerkin2013b](#). The source term arising due to body forces is:

$$\mathcal{U}^S(\rho, \mathbf{v}) = \int_{\Omega} \rho \frac{\mathbf{g}}{\|\mathbf{g}\|} \cdot \mathbf{v} \, dV. \quad (3.35)$$

The right hand sides of Equation (3.26b) and Equation (3.27b) contain the information from Dirichlet boundary conditions:

$$\mathcal{B}^2(\mathbf{v}) = - \oint_{\Gamma_D} \left((\rho \mathbf{u}_D \otimes \mathbf{u}_D) \mathbf{n}_{\Gamma} + \frac{\gamma_1}{2} \mathbf{u}_D \right) \cdot \mathbf{v} \, dS + \oint_{\Gamma_D} \mu_D \mathbf{u}_D \cdot (\nabla_h \mathbf{v} \mathbf{n}_{\Gamma} + \nabla_h \mathbf{v}^T \mathbf{n}_{\Gamma} - \eta \mathbf{v}) \, dS. \quad (3.36)$$

The Dirichlet viscosity value μ_D is calculated from Equation (2.29) using the Dirichlet values of the temperature at the boundary.

Scalar equations Since the convective and diffusive term for the temperature, mass fractions and mixture fraction share a similar form, we summarize here their discretized expressions in terms of an arbitrary scalar X (corresponding to T in the energy equation, Y_α in the equation for species α and z for the mixture fraction equation) and transport parameter ξ (i.e. k/c_p in the energy equation, and (ρD) for the mass fraction and mixture fraction equations). The convective term of the scalars is discretized using a Lax-Friedrichs flux

$$\mathcal{S}^C(\mathbf{u}, X, r, \rho) = \oint_{\Gamma} \left(\{\rho \mathbf{u} X\} \cdot \mathbf{n} + \frac{\gamma_2}{2} [X] \right) [r] \, dS - \int_{\Omega} (\rho \mathbf{u} X \cdot \nabla_h r) \, dV. \quad (3.37)$$

The Lax-Friedrichs parameter γ_2 is calculated as Klein et al., 2016

$$\gamma_2 = \max \left\{ \overline{\rho^+} |\overline{\mathbf{u}^+} \cdot \mathbf{n}^+|, \overline{\rho^-} |\overline{\mathbf{u}^-} \cdot \mathbf{n}^-| \right\}. \quad (3.38)$$

The diffusion term of scalars is discretized again with a SIP formulation:

$$\begin{aligned} \mathcal{S}^D(X, r, \xi) &= \int_{\Omega} (\xi \nabla_h X \cdot \nabla_h r) \, dV \\ &- \oint_{\Gamma \setminus \Gamma_N \setminus \Gamma_{ND}} (\{\xi \nabla_h X\} \cdot \mathbf{n} [r] + \{\xi \nabla_h r\} \cdot \mathbf{n} [X] - \eta \xi_{\max} [X] [r]) \, dS. \end{aligned} \quad (3.39)$$

The transport parameter ξ is calculated as a function of temperature using Equation (2.29) and $\xi_{\max} = \max(\xi^+, \xi^-)$. The boundary condition term of the corresponding scalar equation is:

$$\mathcal{B}^3(r) = - \oint_{\Gamma_D \cup \Gamma_{ND}} \left((\rho_D \mathbf{u}_D X_D) \cdot \mathbf{n}_\Gamma + \frac{\gamma_2}{2} X_D \right) r \, dS + \oint_{\Gamma_D \cup \Gamma_{ND}} \xi_D X_D (\nabla_h r \cdot \mathbf{n}_\Gamma - \eta r) \, dS. \quad (3.40)$$

Here, X_D is the Dirichlet value of the scalar X on boundaries and ξ_D is the corresponding transport parameter calculated, which is calculated with Equation (2.29) using the Dirichlet values of the temperature at the boundary. Finally, the volumetric source term of the energy and mass fraction equations are defined as follows:

$$\mathcal{S}^S(r, Q, \omega, c_p) = \int_{\Omega} \frac{Q\omega}{c_p} r \, dV, \quad (3.41)$$

$$\mathcal{M}_\alpha^S(s_\alpha, \omega) = \int_{\Omega} \nu_\alpha M_\alpha \omega s_\alpha \, dV. \quad (3.42)$$

The heat release Q is calculated with Equation (2.25), the reaction rate ω is evaluated using Equation (2.24) and the mixture heat capacity with Equation (2.28).

3.1.3 Temporal discretization

Blabla second order backward difference scheme

$$\left(\frac{\partial \rho}{\partial t} \right)^n = \frac{1}{2\Delta t} (3\rho^n - 2\rho^{n-1}\rho^{n-2}) \quad (3.43)$$

3.2 Computational methodology

The presented solver is embedded in the *BoSSS* (Bounded Support Spectral Solver) code, which is under development at the chair of fluid dynamics of the Technical University of Darmstadt, and is available under <https://github.com/FDYdarmstadt/BoSSS>. *BoSSS* is a general framework for the discretization of conservation laws using the DG method and uses a modal DG approach with orthonormal Legendre polynomials as basis functions. The *BoSSS* code features a variety of applications in the context of computational fluid dynamics, such as a solver for multiphase flows with a sharp interface approach, Kummer, 2017 an incompressible Immersed Boundary Method solver for particle laden flows,Krause and Kummer, 2017 a solver for viscoelastic fluid flows,Kikker et al., 2020 and a solver for compressible flows, Geisenhofer et al., 2019 among others.

The variational problem for the finite chemistry rate case described by Equations (3.26a) to (3.26d) and for the flame sheet problem, Equations (3.27a) to (3.27c), are linearised and solved using a Newton method with a Dogleg-type globalization Pawłowski et al., 2006; Pawłowski et al., 2008. The *BoSSS* framework provides an efficient algorithm for the evaluation of the Jacobian based on perturbations of the forms presented in the last section. The relatively large linear system of equations for each Newton iteration is solved by means of the in *BoSSS* integrated orthonormalization multigrid algorithm Kummer et al., 2021, which at the lowest multigrid levels makes use of the sparse direct solver PARDISO, originally developed by Schenk et al. Schenk et al., 2000; Schenk and Gärtner, 2002; Schenk and Gärtner, 2004, from the “Intel(R) Parallel Studio XE 2018 Update 3 Cluster Edition for Windows” library collection to solve the linear system.

BoSSS also features a method for solving highly nonlinear problems with a homotopy strategy. Further details on the used Newton method solver, the homotopy strategy and its implementation are given in the next sections, which are adapted from Kikker et al., 2020 and are included for the sake of completeness. For information on the mentioned orthonormalization multigrid algorithm we refer the interested reader to the work of Kummer et al., 2021.

From this point on, the solver presented in this work will be called XNSEC (eXtended Navier-Stokes for Combustion). The term *extended* refers to the framework on which the solver is built, which focuses on applications for multi-phase flows using a sharp interface approach using a level-set method. This point will be briefly discussed in the section

Calculation of the Jacobian matrix

We start by introducing a few new elements to be able to describe the implemented Newton method. The discussion for the variational problem using the mixture fraction variable (Equations (3.27a) to (3.27c)) is completely analogous, and will not be mentioned in this discussions. Find $\mathbf{U}_h \in \mathbb{V}_k$

$$\mathcal{N}(\mathbf{U}_h, \mathbf{V}_h) = 0 \quad \forall \mathbf{V}_h \in \mathbb{V}_k, \quad (3.44)$$

for $\mathbf{U}_h = (p_h, \mathbf{u}_h, T_h, \mathbf{Y}'_h)$ and $\mathbf{V}_h = (q_h, \mathbf{v}_h, r_h, \mathbf{s}_h)$. We assume a basis $\underline{\Phi} = (\Phi_1, \dots, \Phi_L)$ of \mathbb{V}_k , written as a row vector, with $L := \dim(\mathbb{V}_k)$. Then \mathbf{U}_h can be represented as $\mathbf{U}_h = \underline{\Phi} \cdot \mathbf{U}$. The nonlinear problem (3.44) can then be written as

$$\mathcal{A}(\mathbf{U}) = 0, \quad (3.45)$$

with the nonlinear function $\mathbb{R}^L \ni \mathbf{U} \mapsto \mathcal{A}(\mathbf{U}) \in \mathbb{R}^L$. The i -th component of $\mathcal{A}(\mathbf{U})$, can be defined by $\mathcal{N}(-, -)$ through the relation $[\mathcal{A}(\mathbf{U})]_i = \mathcal{N}(\underline{\Phi} \cdot \mathbf{U}, \Phi_i)$.

The formulation of the Newton method requires the Jacobian matrix $\partial\mathcal{A}$ of \mathcal{A} , defined as

$$\partial\mathcal{A}_{ij}(\mathbf{U}) := \frac{\partial\mathcal{A}_i}{\partial U_j}(\mathbf{U}). \quad (3.46)$$

Its computation is quite straightforward, but lengthy. The *BoSSS* code is capable of evaluating the Jacobian matrix automatically from the expressions given in Section 3.1.1. We note that one could write $\mathcal{A}(\mathbf{U})$ as

$$[\mathcal{A}(\mathbf{U})]_i = \mathcal{N}(\mathbf{U}_h, \Phi_i) = \int_{\Omega_h} N_1(\mathbf{x}, \mathbf{U}_h, \nabla \mathbf{U}_h) \cdot \Phi_i + N_2(\mathbf{x}, \mathbf{U}_h, \nabla \mathbf{U}_h) \cdot \nabla \Phi_i dV + \oint_{\Gamma} \dots dS. \quad (3.47)$$

The edge integral, which is left out in Equation (3.47), can be written in analogous fashion as the volume integral, i.e. as a sum over four nonlinear functions, multiplied by Φ_i^+ , Φ_i^- , $\nabla \Phi_i^+$ and $\nabla \Phi_i^-$, respectively. These functions themselves may depend on \mathbf{x} , \mathbf{U}_h^+ , \mathbf{U}_h^- , $\nabla \mathbf{U}_h^+$ and $\nabla \mathbf{U}_h^-$. For sake of compactness, this part is skipped. Realizing that $\frac{\partial \mathbf{U}_h}{\partial U_j} = \Phi_j$ and by application of the chain rule, one derives

$$\partial\mathcal{A}_{ij}(\mathbf{U}) = \int_{\Omega_h} (\partial_{\mathbf{U}_h} N_1(\mathbf{x}, \mathbf{U}_h, \nabla \mathbf{U}_h) \Phi_j + \partial_{\nabla \mathbf{U}_h} N_1(\mathbf{x}, \mathbf{U}_h, \nabla \mathbf{U}_h) \nabla \Phi_j) \cdot \Phi_i + \dots dV + \oint_{\Gamma} \dots dS. \quad (3.48)$$

All skipped terms in Equation (3.48) can be derived in an analogous fashion as the contributions for N_1 . In the *BoSSS* code, derivatives $\partial_{\mathbf{U}_h} N_1(\dots)$ and $\partial_{\nabla \mathbf{U}_h} N_1(\dots)$ are approximated by a finite difference, using a perturbation by $\sqrt{\text{eps}}$ in the respective argument, where $\text{eps} = 2.22044604925031 \cdot 10^{-16}$ is the floating point accuracy for double precision.

The notation introduced here allows us to describe the Newton-Dogleg method used in this work. We note however that this globalization strategy is still not sufficient to ensure convergence for some of the test cases presented, namely for high Rayleigh numbers for the differentially heated cavity problem. For those cases we use a homotopy strategy, where we start with a low homotopy-parameter, a parameter for which the solution of the problem is not hard to find, which is gradually and carefully increased until convergence for the desired value of the homotopy-parameter is reached (cf. Section 3.2.4).

3.2.1 Dogleg Method

We consider a linearization of Equation (3.45) around \mathbf{U}_n ,

$$\mathcal{A}(\mathbf{U}_n) + \partial\mathcal{A}(\mathbf{U}_n) \underbrace{(\mathbf{U}_{n+1} - \mathbf{U}_n)}_{=: \mathbf{s}'_n} = 0. \quad (3.49)$$

By repeatedly solving this system one obtains a standard Newton scheme for Equation (3.45), yielding a sequence of approximate solutions $\mathbf{U}_0, \mathbf{U}_1, \mathbf{U}_2, \dots$ obtained from an initial guess \mathbf{U}_0 through the iteration scheme $\mathbf{U}_{n+1} = \mathbf{U}_n + \mathbf{s}'_n$. In the classical un-damped Newton method, the correction step \mathbf{s}'_n is set to be the whole Newton-step, i.e $\mathbf{s}'_n = \mathbf{s}_n$ with

$$\mathbf{s}_n := -\partial\mathcal{A}(\mathbf{U}_n)^{-1} \mathcal{A}(\mathbf{U}_n), \quad (3.50)$$

which is computed using a direct solver. Unfortunately, convergence of the Newton method for any starting value \mathbf{U}_0 is not guaranteed. In order to increase robustness when the distance between \mathbf{U}_0 and the exact solution \mathbf{U} is large, we employ a globalization approach, presented by

Pawlowski et al. Pawlowski et al., 2006; Pawlowski et al., 2008, known as the Dogleg-method, or Newton-Dogleg method. Here, we intend to give only the central ideas of method and refer to the original works for further details. Obviously, the exact solution of Equation (3.45) is also a minimum of the functional

$$f(\mathbf{U}) := \frac{1}{2} \|\mathcal{A}(\mathbf{U})\|_2^2. \quad (3.51)$$

One observes that $\nabla f(\mathbf{U}) = \partial\mathcal{A}(\mathbf{U})^T \mathcal{A}(\mathbf{U})$. For \mathbf{U}_n , the approximate Cauchy point with respect to the 2-norm, is defined as the minimizer \mathbf{g}_n of $\|\mathcal{A}(\mathbf{U}_n) + \partial\mathcal{A}(\mathbf{U}_n)\mathbf{g}_n\|_2$ in the direction of steepest decent, i.e. $\mathbf{g}_n = \lambda \nabla f(\mathbf{U}_n)$, $\lambda \in \mathbb{R}$. Substituting $\mathbf{w} := -\partial\mathcal{A}(\mathbf{U}_n) \nabla f(\mathbf{U}_n)$, \mathbf{g}_n is given by

$$\mathbf{g}_n = \frac{\mathcal{A}(\mathbf{U}_n) \cdot \mathbf{w}}{\mathbf{w} \cdot \mathbf{w}} \nabla f(\mathbf{U}_n). \quad (3.52)$$

For the Newton-Dogleg method, the correction step \mathbf{s}'_n is chosen along the so-called Dogleg curve, which is the piece-wise linear curve from the origin to \mathbf{g}_n and further to \mathbf{s}_n . The selection of \mathbf{s}'_n on this curve is determined by the trust-region diameter $\delta > 0$:

- If $\|\mathbf{s}_n\|_2 \leq \delta$, $\mathbf{s}'_n = \mathbf{s}_n$.
- If $\|\mathbf{g}_n\|_2 \leq \delta$ and $\|\mathbf{s}_n\|_2 > \delta$, \mathbf{s}'_n is chosen on the linear interpolation from \mathbf{g}_n to \mathbf{s}_n so that $\|\mathbf{s}'_n\|_2 = \delta$: For the ansatz $\mathbf{s}'_n = \tau \mathbf{s}_n + (1 - \tau) \mathbf{g}_n$, the interpolation factor τ is given as $\tau = (a^2 - c + \sqrt{(a^2 + b^2 - 2c)\delta^2 - a^2b^2 + c^2})/(a^2 + b^2 - 2c)$ with $a = \|\mathbf{g}_n\|_2$, $b = \|\mathbf{s}_n\|_2$ and $c = \mathbf{g}_n \cdot \mathbf{s}_n$.
- If $\|\mathbf{g}_n\|_2 > \delta$, $\mathbf{g}_n = (\delta/\|\mathbf{g}_n\|_2)\mathbf{g}_n$.

The choice and adaptation of the trust region diameter δ throughout the Newton-Dogleg procedure follows a sophisticated heuristic, mainly based on comparing the actual residual reduction $\text{ared}_n := \|\mathcal{A}(\mathbf{U}_n)\|_2 - \|\mathcal{A}(\mathbf{U}_n + \mathbf{s}'_n)\|_2$ with the predicted residual reduction $\text{pred}_n := \|\mathcal{A}(\mathbf{U}_n)\|_2 - \|\mathcal{A}(\mathbf{U}_n) + \partial\mathcal{A}(\mathbf{U}_n)\mathbf{s}'_n\|_2$; For the direct solver used in this work pred_n simplifies to $\text{pred}_n := \|\mathcal{A}(\mathbf{U}_n)\|_2$. We replicate the algorithm here, for the sake of completeness:

- (1) Set $n = 0$, $\delta_n = \min(10^{10}, \max(2 \cdot 10^{-6}, \|\mathbf{s}_0\|_2))$.
- (2) Compute the Newton step \mathbf{s}_n and the Cauchy point \mathbf{g}_n and find \mathbf{s}'_n on the Dogleg curve with respect to the recent δ_n .
- (3) While $\text{ared}_n \leq \text{pred}_n$ do: Update trust region diameter $\delta_n \leftarrow 0.5 \delta_n$ and re-compute \mathbf{s}'_n . If $\delta_n < 10^{-6}$ terminate abnormally and mark the computation as failed.
- (4) If the convergence criterion (see below) is fulfilled, terminate and mark the computation as success.
- (5) Perform a final update of the trust region: Set

$$\delta_{n+1} = \begin{cases} \max(10^{-6}, \|\mathbf{s}_n\|_2) & \text{if } \text{ared}_n/\text{pred}_n < 0.1 \text{ and } \|\mathbf{s}_n\|_2 \delta_n \\ \max(10^{-6}, 0.25 \cdot \delta_n) & \text{else, if } \text{ared}_n/\text{pred}_n < 0.1 \\ \min(10^{10}, 4 \cdot \delta_n) & \text{else, if } \text{ared}_n/\text{pred}_n > 0.75 \\ \delta_n & \text{otherwise} \end{cases}$$

Set $\mathbf{U}_{n+1} = \mathbf{U}_n + \mathbf{s}'_n$, update $n \leftarrow n + 1$ and return to step (2).

All constants used in the algorithm above have been taken from the work of Pawlowski et al. Pawlowski et al., 2006 For a detailed description of the underlying ideas we also refer to these works, which in turn are based on algorithms from Dennis and Schnabel's textbook. Dennis and Schnabel, 1996

3.2.2 Termination criterion

A simple approach to determine that a Newton-Dogleg loop can be terminated is to check whether the residual norm has fallen below a certain threshold, i.e. $\|\mathcal{A}(U_n)\| \leq \text{tol}$. A universal choice for the tolerance is indeed difficult, especially for investigations of convergence properties (cf. Section 4.2.3 and Section 4.3.3). If it is chosen too low, the algorithm may never terminate, because of dominating numerical round-off errors. On the other hand, if it is chosen too high, the error of the premature termination may dominate the error of the spatial discretization and one cannot take the full advantage of the high-order method. Therefore the goal is to continue the Newton-Dogleg method until the lowest possible limit dictated by floating point accuracy is reached. To identify the limit in a robust way, we first define the residual-norm skyline as

$$\text{sr}_n := \min_{j \leq n} \|\mathcal{A}(\mathbf{U}_j)\| \quad (3.53)$$

and, for $n \geq 2$, the averaged reduction factor

$$\text{arf}_n := \frac{1}{2} \left(\frac{\text{sr}_{n-2}}{\max\{\text{sr}_{n-1}, 10^{-100}\}} + \frac{\text{sr}_{n-1}}{\max\{\text{sr}_n, 10^{-100}\}} \right). \quad (3.54)$$

The Newton-Dogleg method is terminated if

$$n \geq 2 \text{ and } \text{sr}_n \leq 10^{-5} + 10^{-5} \|\mathbf{U}_n\|_2 \text{ and } \text{arf}_n < 1.5. \quad (3.55)$$

For the computations in this work, this choice guarantees that the nonlinear system is solved as accurately as possible. It secures that the numerical error is dominated by the error of the spatial or temporal discretization and not by the termination criterion of the Newton-Dogleg method. The skyline approach ensures robustness against oscillations close to the lower limit.

3.2.3 Solver safeguard

/// 'safeguard' for solvers to avoid unphysical solutions during the solution procedure; /// An example would be to avoid e.g. negative densities, which might even cause NaNs, /// during the solver run for implicit, nonlinear equations.

3.2.4 Homotopy method

Although the Newton-Dogleg method works well for a variety of cases, we experienced convergence problems for some of the test cases presented in next section. In particular, for the differentially heated cavity test case, the method was not successful on finding a convergent solution for a Rayleigh number $Ra \geq 10^5$ within 60 Newton iterations. In such cases we used a homotopy strategy, which is loosely based on ideas from the textbook of Deuflhard, Deuflhard, 2011 Chapter 5.

We start by identifying a parameter that makes the solution of the nonlinear problem difficult to solve. In the following we will refer to this variable as the homotopy parameter. The main

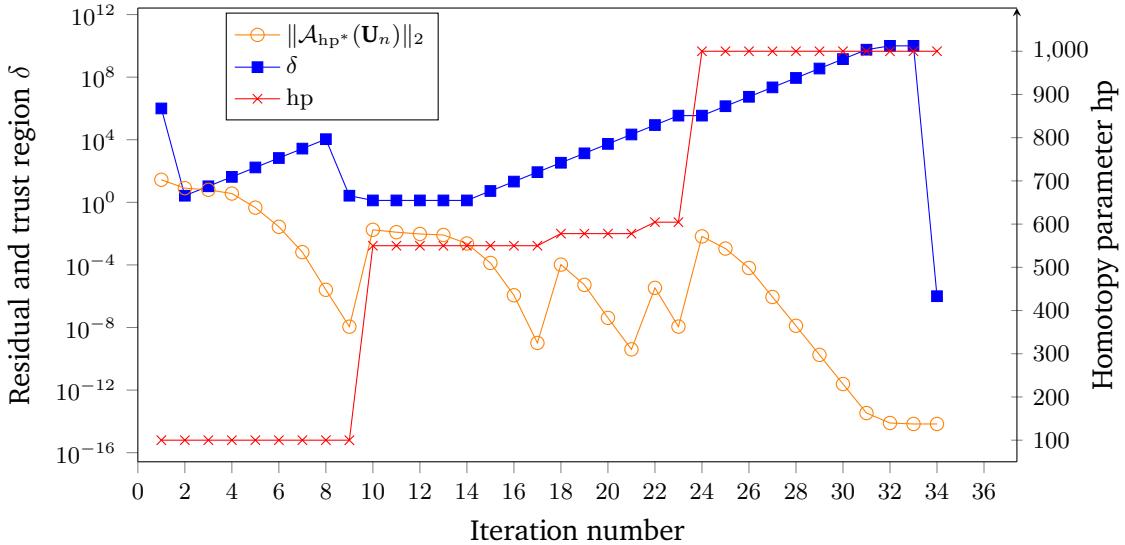


Figure 3.1: Behaviour of the homotopy method for the differentially heated cavity test case. The homotopy parameter hp in this case is the Reynolds number.

idea of the homotopy strategy consists of solving a series of simpler problems, starting with a parameter where the problem is easy to solve, and carefully increasing it until the desired value is reached. Let Hp denote the value of the homotopy parameter for which a solution is being sought. Let

$$\mathcal{A}_{hp^*}(\mathbf{U}) = 0 \quad (3.56)$$

be the discretized system for a certain intermediate homotopy-parameter hp^* , between 0 and the ‘target’ homotopy-parameter Hp , i.e. $0 \leq hp^* \leq Hp$. Furthermore, let $\mathbf{U}_{hp,\epsilon}$ be an approximate solution to the problem (3.56) with $hp^* = hp$, up to a tolerance ϵ , i.e.

$$\|\mathcal{A}_{hp}(\mathbf{U}_{hp,\epsilon})\|_2 \leq \epsilon. \quad (3.57)$$

For the sake of clarity when discussing the algorithm which follows below, we distinguish between the intermediate homotopy-parameter hp for which we assume to already have found an acceptable solution and the next homotopy-parameter hp^* that we are currently trying to find a solution for. For any $hp^* > hp$ we set $\epsilon = 10^{-5} \|\mathcal{A}_{hp^*}(\mathbf{U}_{hp,\epsilon})\|_2$, i.e. we aim for a residual norm reduction of at least five orders of magnitude with respect to the initial residual norm. If $hp^* = Hp$, the termination criterion presented in section 3.2.2 is applied. An approximate solution for the target homotopy-parameter is found by the following recipe:

- (1) Set $hp = 0$, i.e. start by obtaining an (approximate) solution $\mathbf{U}_{0,\epsilon}$.
- (2) Search for a an increased homotopy-parameter hp^* : Find the minimal $i \geq 0$ so that for $hp^* = \frac{1}{2^i}(Hp - hp) + hp$ one has $\|\mathcal{A}_{hp^*}(\mathbf{U}_{hp,\epsilon})\|_2 \leq \delta_{\max} \|\mathcal{A}_{hp}(\mathbf{U}_{hp,\epsilon})\|_2$. Here, δ_{\max} is the maximal allowed increase of the residual for an increased homotopy-parameter hp^* ; δ_{\max} is adapted in the following steps, as an initial guess we use $\delta_{\max} = 10^6$.
- (3) Use the Newton-Dogleg method to compute an approximate solution to the problem (3.56), for the homotopy-parameter hp^* , using the solution $\mathbf{U}_{hp,\epsilon}$ as an initial guess.

- If the Newton-Dogleg method did not converge successfully within ten steps, the homotopy-parameter increase from hp to hp^* was probably too large. Set $\delta_{\max} \leftarrow 0.2\delta_{\max}$ and go to step (2).
- If the Newton-Dogleg method reached its convergence criterion and if the target homotopy-parameter is reached, i.e. $hp^* = Hp$, the algorithm has successfully found an approximate solution for $\mathcal{A}_{Hp}(\mathbf{U}) = 0$ and can terminate.
- Otherwise, if the Newton-Dogleg method converged successfully, but is below the target homotopy-parameter: Accept the solution and set $hp \leftarrow hp^*$. If the Newton-Dogleg method took less than three iterations to reach the convergence criterion, set $\delta_{\max} \leftarrow 8\delta_{\max}$. Return to step (2).

An exemplary run of the method is shown in Figure 3.1. The homotopy parameter hp in this particular case is the Reynolds number. The homotopy-parameter hp was increased for iterations 10, 18, 22 and 24, causing an increase of the residuals $\|\mathcal{A}_{hp^*}(\mathbf{U}_n)\|_2$, leading to a convergent solution after 34 Newton iterations. The presented algorithm offers a robust method for finding steady-state solutions of highly nonlinear systems.

3.2.5 Initialization of combustion applications

Cases involving combustion are initialized with the solution of the flame sheet problem, Equations (3.27a) to (3.27c). This idea has been already employed in various works. Smooke et al., 1986; Smooke and Giovangigli, 1992 The reason for the use of this pre-step is twofold:

- Solving **????** and Equations (2.22c) and (2.22d) using a Newton-type method requires adequate starting estimates in order to converge. Using the flame sheet solution as initial estimate improves the convergence properties of the method.
- The system of **????** and Equations (2.22c) and (2.22d) possesses multiple solutions. One is the pure mixing (frozen) solution, where no chemical reaction has taken place, and the other one is the ignited solution, where the flame is present. Using the flame sheet solution as initial estimate ensures that the path taken by Newton's algorithm will tend towards the ignited solution.

It should be noted regarding the solution of the flame sheet problem (cf. Section 2.2) that the sharp change in the primitive variables around $z = z_{st}$ is problematic in certain scenarios. In particular, the non-smoothness of the derived variables could lead to Gibbs phenomenon-type problems. This inconvenient can be remedied by using a regularized form of the equations. The smoothing function \mathcal{H} is defined as

$$\mathcal{H}(z) \approx \frac{1}{2}(1 + \tanh(\frac{z - z_{st}}{\sigma})), \quad (3.58)$$

This function is useful for creating a smooth transition between two functions, since it returns values close to 0 for $z \ll z_{st}$ and values close to 1 for $z \gg z_{st}$. The sharpness of the transition at the point $z = z_{st}$ is dictated by the parameter σ . In Figure 3.4 the effect of the smoothing factor σ on calculations of a flame in a counter-flow configuration are shown. It can be clearly observed how for increasing σ the solution becomes smoother. Using Equation (3.58)

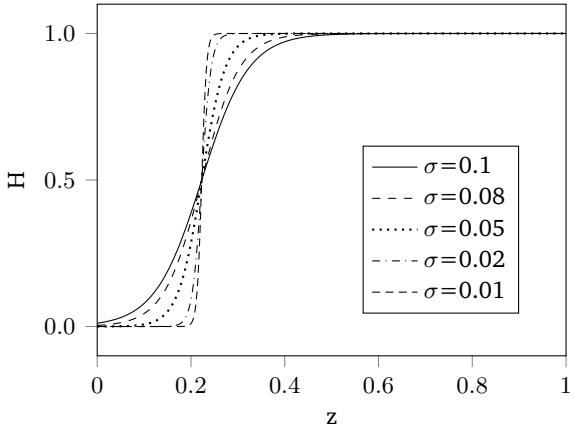


Figure 3.2: Smoothing function for different σ and z_{st}

the temperature and mass fraction fields can be written as

$$T(z) = zT_F^0 + (1 - z)T_O^0 + \frac{QY_F^0}{c_p} z_{st} \frac{1 - z}{1 - z_{st}} \mathcal{H}(z) + \frac{QY_F^0}{c_p} z (1 - \mathcal{H}(z)), \quad (3.59a)$$

$$Y_F(z) = Y_F^0 \frac{z - z_{st}}{1 - z_{st}} \mathcal{H}(z), \quad (3.59b)$$

$$Y_O(z) = Y_O^0 \frac{z_{st} - z}{z_{st}} (1 - \mathcal{H}(z)), \quad (3.59c)$$

$$Y_P(z) = Y_O^0 \frac{M_P \nu_P}{M_O \nu_O} (1 - z) \mathcal{H}(z) + Y_F^0 \frac{M_P \nu_P}{M_F \nu_F} z (1 - \mathcal{H}(z)), \quad (3.59d)$$

$$Y_N(z) = (1 - Y_F^0)z + (1 - Y_O^0)(1 - z). \quad (3.59e)$$

The use of this regularized form of the equations results in practice on a spreading of the flame front, which eases the numerical calculation (Braack et al., 1997).

One question one could certainly ask is under what flame conditions is the infinite reaction-rate solution (also called flame-sheet solution in the following) effectively a good initial estimate for Newton's algorithm. Recall that for the derivation of the

Although for the solution of the infinite reaction rate system the mixture heat capacity has been assumed to be constant, it remains an adequate estimate for the finite reaction-rate problem, where the heat capacity is a function of temperature and local concentration. In a similar fashion, the assumption of unity Lewis number in the flame sheet system delivers a solution that slightly deviates from the solution of the finite chemistry rate problem with non-unity Lewis numbers. Nevertheless, this small deviation does not preclude the use of the flame sheet solution as an adequate initial estimate for Newton's method.

One problem that arises when using the flame sheet estimate is the selection of a suitable c_p , since the flame temperature - and therefore all other solution fields - are highly dependent on the selection of the heat capacity. Xu and Smooke, 1993 suggests estimating it simply on the basis of experimental measurements, or also by selecting some representative value.

It should also be noted that crefeq:heatReleaseOneStep yields unphysical values of \hat{Q} for large values of ϕ . This problem can be avoided by setting an upper boundary value for ϕ in Equation (2.20) (we use $\phi = 1.2$). In practice however, this should not have a significant effect,

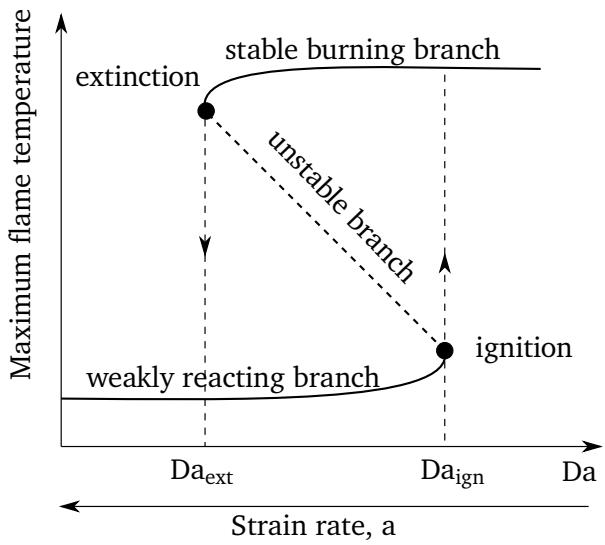


Figure 3.3: S-shaped bifurcation curve of a combustion process.

because the unphysical values of \hat{Q} appear at zones where the reaction rate $\hat{\omega}$ is very close to zero, making the factor $\hat{Q}\hat{\omega}$ in the temperature equation negligible. Nevertheless, setting an upper bound for ϕ is helpful to avoid possible numerical instabilities.

Adaptive Mesh Refinement

The area where the chemical reaction takes place is usually a thin region whose thickness is defined by the availability of reactants.

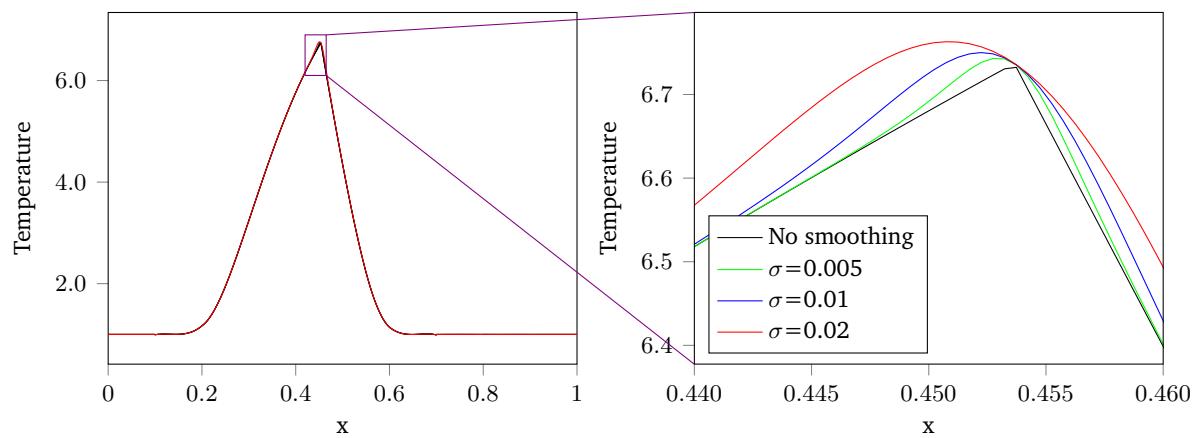


Figure 3.4: Temperature profile calculated in the center-line of a counter-flow flame configuration for different smoothing parameters σ .

4 Results

The following sections show a comprehensive solver validation using various test cases presented in increasing levels of complexity. The tests also allow to highlight some of the benefits of the DG-method and the algorithms introduced before in this work, namely the globalized Newton method, homotopy strategy and the initialization of combustion applications using flame-sheet estimates.

First, in Section 4.1 the applicability of the solver is analyzed for isothermal single-component systems. Later in Section 4.2 several single-component non-isothermal configurations are studied. Finally, in Section 4.3 test cases for multicomponent non-isothermal systems are presented, with a particular emphasis on systems where combustion is present.

All calculations shown here were performed on a cluster with the following specifications.

- CPU 4x8 cores (Intel(R) Xeon(R) CPU E5-4627 v2)
- CPU vector extension Intel® AVX
- CPU speed basis 3.30 GHz, turbo 3.6 GHz
- memory 512 GByte (DDR3-1600)

Unless otherwise stated, all calculations use the termination criteria presented in Section 3.2.2. Some of the results presented in the next sections has been published (Gutiérrez-Jorquera and Kummer, 2022).

4.1 Single-component isothermal cases

The XNSEC-solver presented in the previous chapter is validated first for single-component isothermal cases. In these cases, only the continuity and momentum equations are solved. The energy equation and the species concentration equations are replaced by the conditions $T = 1.0$ and $Y_0 = 1.0$ in the entire domain. This means that the physical properties of the flow (density and viscosity) are constant and that the flow is fully incompressible because the density does not show a thermodynamic or hydrodynamic dependence.

4.1.1 Lid-driven cavity flow

The lid-driven cavity flow is a classically used test problem for the validation of Navier-Stokes solvers. The system configuration is shown in Figure 4.1. It consists simply of a two-dimensional square cavity enclosed by walls whose upper boundary moves at constant velocity, causing the fluid to move. Benchmark results can be found widely in the literature for different Reynolds numbers. In this section, the results obtained with the XNSEC-Solver are compared with those published by Botella and Peyret, 1998.

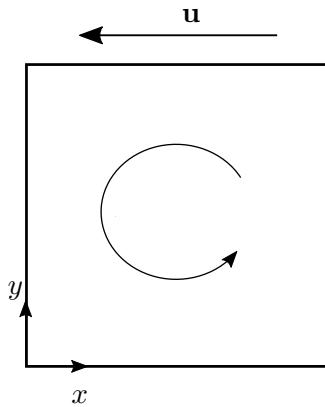


Figure 4.1: Schematic representation of the Lid-Driven cavity flow.

The problem is defined in the domain $\Omega = [0, 1] \times [0, 1]$. The system is solved for the velocity vector $\mathbf{u} = (u, v)$ and the pressure p . All boundary conditions are Dirichlet-type, particularly with $\mathbf{u} = (-1, 0)$ for the boundary at $y = 1$ and $\mathbf{u} = (0, 0)$ for all other sides. The gravity vector is set to $\mathbf{g} = (0, 0)$. A Cartesian mesh with extra refinement at both upper corners is used, and is shown in Figure 4.2. The refinement was done to better represent the complex effects that take place in the corners. The streamline plot presented in Figure 4.2 shows the different vortex structures typical of this kind of system, where in addition to the main vortex of the cavity, smaller structures appear in the corners.

The lid-driven cavity was calculated for a Reynolds number $Re = 1000$. For the calculations presented here, the polynomial degree is set to $k = 4$ and $k' = 3$. A regular Cartesian mesh with 16×16 elements is used with extra refinement in the corners. In Figure 4.3 a comparison of the calculated velocity with the DG-Solver and the velocities provided by the benchmark is shown. Clearly, very good agreement is obtained, even by using a relatively coarse mesh (the benchmark result uses a grid with 160×160 elements).

A more rigorous comparison of results is presented in Table 4.1, where the extreme values of the velocity components calculated through the centerline of the cavity are compared with the results presented by Botella and Peyret, 1998. Different mesh resolutions were used for

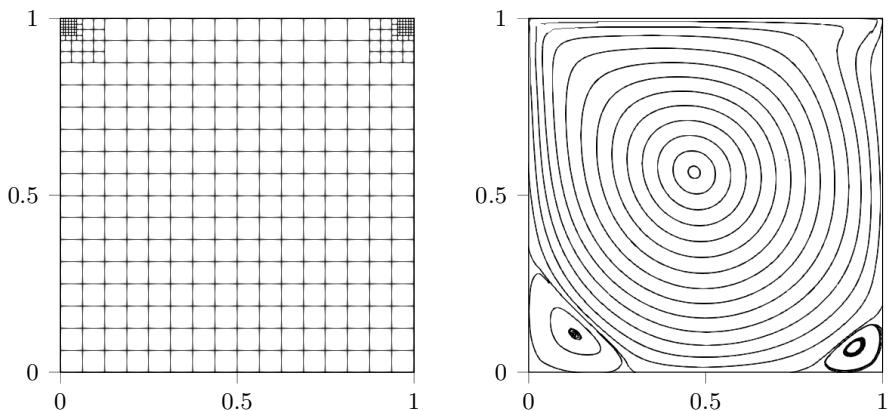


Figure 4.2: Mesh and streamlines of the lid-driven cavity flow with $Re = 1000$

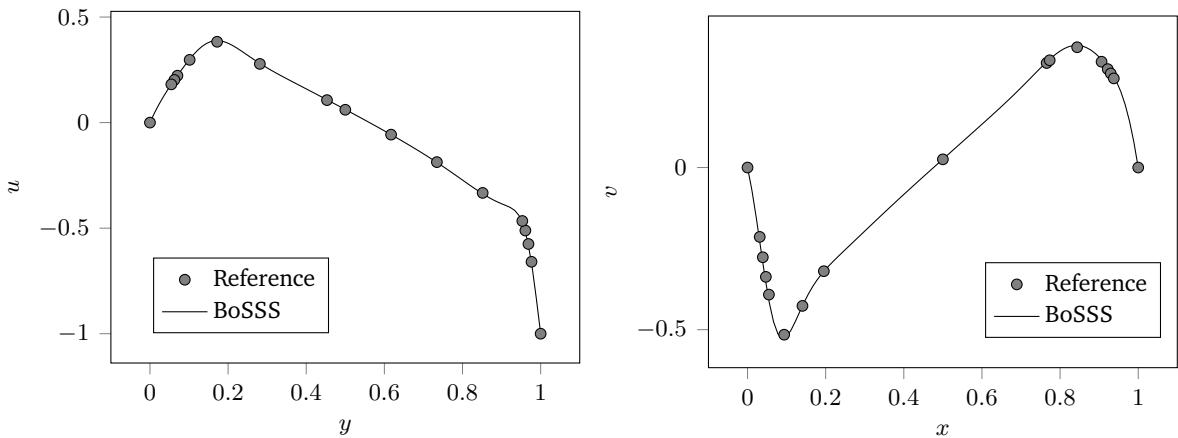


Figure 4.3: Calculated velocities along the centerlines of the cavity and reference values. Left plot shows the x-velocity for $x = 0.5$. Right plot shows the y-velocity for $y = 0.5$

Mesh	u_{\max}	y_{\max}	v_{\max}	x_{\max}	v_{\min}	x_{\min}
16×16	0.3852327	0.1820	0.3737295	0.8221	-0.5056627	0.0941
32×32	0.3872588	0.1821	0.3760675	0.8227	-0.5080496	0.0943
64×64	0.3897104	0.1748	0.3774796	0.8408	-0.5248360	0.0937
128×128	0.3886452	0.1720	0.3770127	0.8422	-0.5271487	0.0907
256×256	0.3885661	0.1717	0.3769403	0.8422	-0.5270653	0.0907
Reference	0.3885698	0.1717	0.3769447	0.8422	-0.5270771	0.0908

Table 4.1: Extrema of velocity components through the centerlines of the lid-driven cavity for $\text{Re} = 1000$. Reference values obtained from Botella and Peyret, 1998

this comparison, particularly meshes with 16×16 , 32×32 , 64×64 , 128×128 and 256×256 elements, each with extra refinement at the corners. It can be clearly seen how for the finest mesh the results obtained with the DG-solver are extremely close to the reference, seeing a difference only at the fifth digit after the decimal point for the velocity components, and no difference for the spatial coordinates where the extrema are. It can also be appreciated that the results obtained with the coarser meshes are still very close to those of the reference. It is worth mentioning that this comparison only considering number of elements could be considered unfair, since the reference uses another method for solving the governing equations. One of the advantages of the DG method is that choosing higher-order polynomials allows more information to be packed into each cell. A better comparison would be achieved by comparing results based on the number of degrees of freedom(dofs) used in the simulation, as will be done later in section

4.1.2 Backward-facing step

The backward-facing step problem is another classical configuration widely used for validation of incompressible CFD codes. It has been widely studied theoretically, experimentally, and numerically by many authors in the last decades (see, for example, Armaly et al., 1983; Barkley et al., 2000; Biswas et al., 2004). In Figure 4.4 a schematic representation of the problem is shown. It consists of a channel flow (usually considered fully developed) that is subjected to a

sudden change in geometry that causes separation and reattachment phenomena. For these reasons, this case can be considered more challenging than the one presented in the previous section, since special care of the mesh used has to be taken in order to capture accurately all complex phenomena taking place.

Although the backward-facing step problem is known to be inherently three-dimensional, it has been shown that it can be studied as a two-dimensional configuration along the symmetry plane for moderate Reynolds numbers. For the range of Reynolds numbers used in the calculations presented here, the two-dimensional assumption is justified (Barkley et al., 2000; Biswas et al., 2004). The origin of the coordinate system is set in the bottom part of the step. The step height S and channel height h characterize the system. Results in the literature are often reported as a function of the expansion ratio, defined as $ER = (h + S)/h$.

A series of simulations were performed with the objective of reproducing the results reported by Biswas et al., 2004, where the backward-facing step was calculated for Reynolds numbers up to 400 and for an expansion ratio of 1.9423. In particular, the reported lengths of deattachment and reattachment are used as a means of comparison with the results from the XNSEC-solver.

The Reynolds number for the backward-facing step configuration is defined in the literature in many forms. Here, the definition based on the step height \hat{S} and the mean inlet velocity \hat{U}_{mean} is adopted as the reference length and velocity, resulting in

$$Re = \frac{\hat{S}\hat{U}_{\text{mean}}}{\hat{\nu}}. \quad (4.1)$$

The boundary at $x = -L_0$ is an inlet boundary condition, where a parabolic profile is defined with

$$u(y) = -6 \frac{(y - S)(y - (h + S))}{h^2} \quad (4.2)$$

The system is isothermal, and the fluid is assumed to be air. The step length is set $S = 1$ and $h = 1.061$. To minimize the effects of the outlet boundary condition on the part of interest in the system, the length L of the domain is set to $L = 70S$. All other boundaries are fixed walls. From prior calculations, the effect of the domain length before the step was found to have almost no impact on the results and is set to $L_0 = S$. Preliminary calculations showed that the calculated reattachment and detachment lengths are highly sensitive to the mesh resolution. For all calculations in this section, a structured grid with 88400 elements is used. To better resolve the complex structures that occur in this configuration, smaller elements are used in the vicinity of the step, as seen in Figure 4.5. A polynomial degree of three was chosen for both velocity components and two for pressure.

The backward-facing step configuration exhibits varying behavior as the number of Reynolds changes. For small Reynolds numbers, a single vortex, usually called the primary vortex, appears in the vicinity of the step. Furthermore, as the Reynolds number increases, a second vortex eventually appears on the top wall, as shown schematically in Figure 4.4. The detachment and reattachment lengths of the vortices are values that are usually reported in the literature. It is possible to determine the detachment position by finding the point along the wall where the velocity gradient normal to the wall acquires a value equal to zero.

Figure 4.7 shows the detachment and reattachment lengths of the primary and secondary vortices obtained with the XSEC solver for different Reynolds numbers, which are also compared with the results presented in the reference paper from Biswas et al., 2004. Cubic splines have been used to accurately locate this point. It can be seen that the results for the detachment lengths of the primary vortex R_1 are in very good agreement with those of the

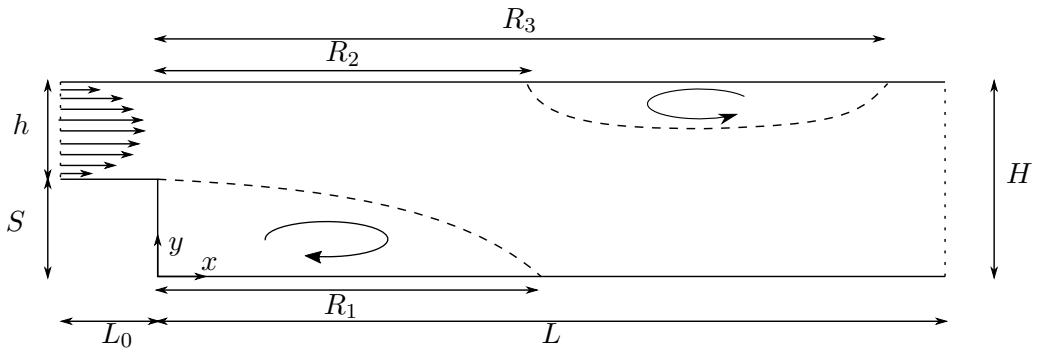


Figure 4.4: Schematic representation (not to scale) of the backward-facing step. Both primary and secondary vortices are shown.

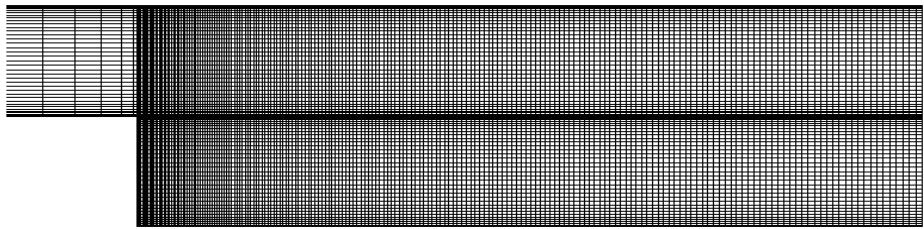


Figure 4.5: Mesh used for the backward-facing step configuration.

reference. In the case of the secondary vortex, it is possible to see a very minimal deviation for the lengths of the reattachment R_3 , hinting at a possible spatial underresolution far away from the step. It is interesting to note that, despite the fact that the reference does not report the existence of a secondary vortex for $\text{Re} = 200$, it was possible to observe it with the XNSEC-solver. The results allow us to conclude that it is possible to study flows with complex behavior for low- to moderate Reynolds numbers, at least in the isothermal case. In the next section, a non-isothermal case of this configuration will be studied.

It is worth mentioning that the evaluation of the global order of accuracy of the solver using the two incompressible test cases presented in this section is problematic due to the presence of singularities, specifically at the corners at the coordinates $\mathbf{x} = (0, 1)$ and $\mathbf{x} = (1, 1)$ of the Lid-driven cavity (where the pressure is not finite according to Botella and Peyret, 1998), and at the corner of the step $\mathbf{x} = (0, S)$ of the backward-facing step. The accuracy of the solver will be assessed later in Section 4.2.2 making use of a analytical solution and Section 4.2.3 using a solution obtained with a high spatial resolution.

4.2 Single-component non-isothermal cases

For the test cases presented in this section, the equations for continuity, momentum and energy are solved. All systems are assumed to be single-component, thus $N = 1$ and $Y_0 = 1.0$. The tests shown in this section shall serve as a throughout validation of the XNSEC-solver spatial and temporal discretization for low-Mach variable density flows.

First in Section 4.2.1 an extension of the backward-facing step configuration for a non-isothermal system is shown, and benchmark values are compared to references. Later in

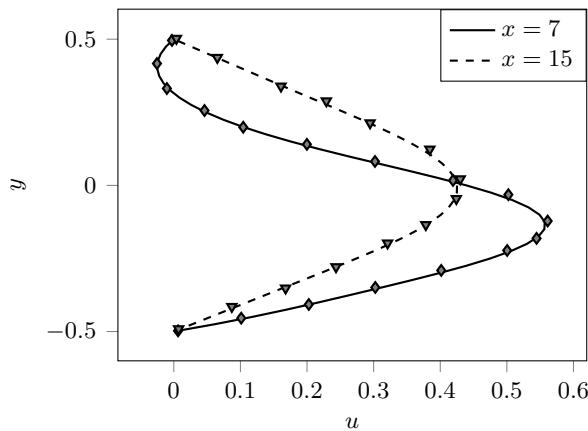


Figure 4.6: Distribution of x-component of velocity in the backward-facing step configuration for a Reynolds number of 400. Solid lines correspond to results obtained with the XNSEC solver.

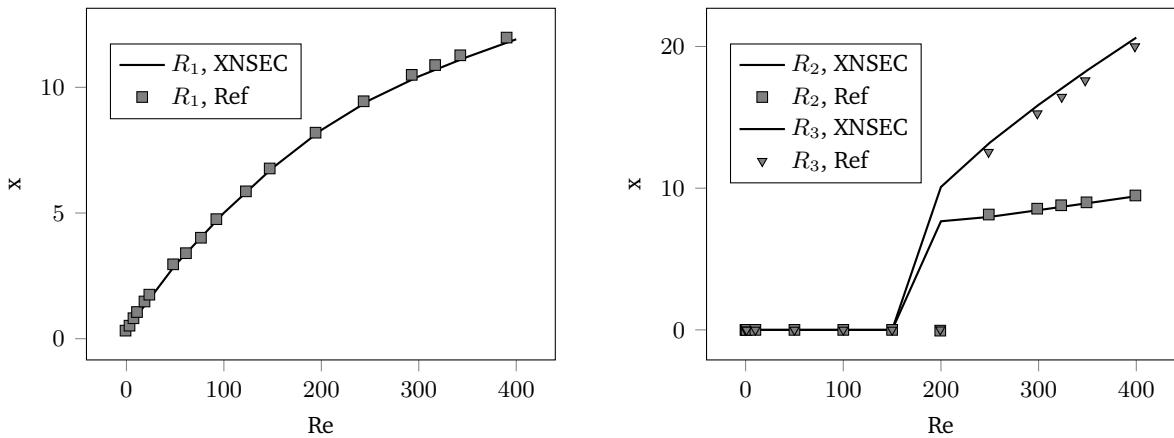


Figure 4.7: Detachment and reattachment lengths of the primary (left figure) and secondary (right figure) recirculation zones after the backward-facing step compared to the reference solution (Biswas et al., 2004).

Section 4.2.2 a Couette flow configuration that presents a temperature gradient in the vertical direction is studied and compared to an analytical solution. Additionally the numerical accuracy of the solver is shown and compared to calculations using a SIMPLE-type algorithm. Later in Section 4.2.3 a heated square cavity configuration is studied to assess the solver's ability to simulate steady state flow configurations of variable density in closed systems. In Section 4.2.4 the flow over a heated cylinder is studied, which serves as a test for unsteady calculations of non-isothermal systems. Finally in Section 4.2.5 a classical Rayleigh-Bénard convection system is treated, showing the behaviour of the solver for instable systems.

4.2.1 Heated backward-facing step

As an extension to the previous case the backward-facing step configuration in a non-isothermal configuration is studied, where the bottom wall is heated to a constant temperature.

In this section the configuration for a heated backward-facing step proposed in Xie and Xi,

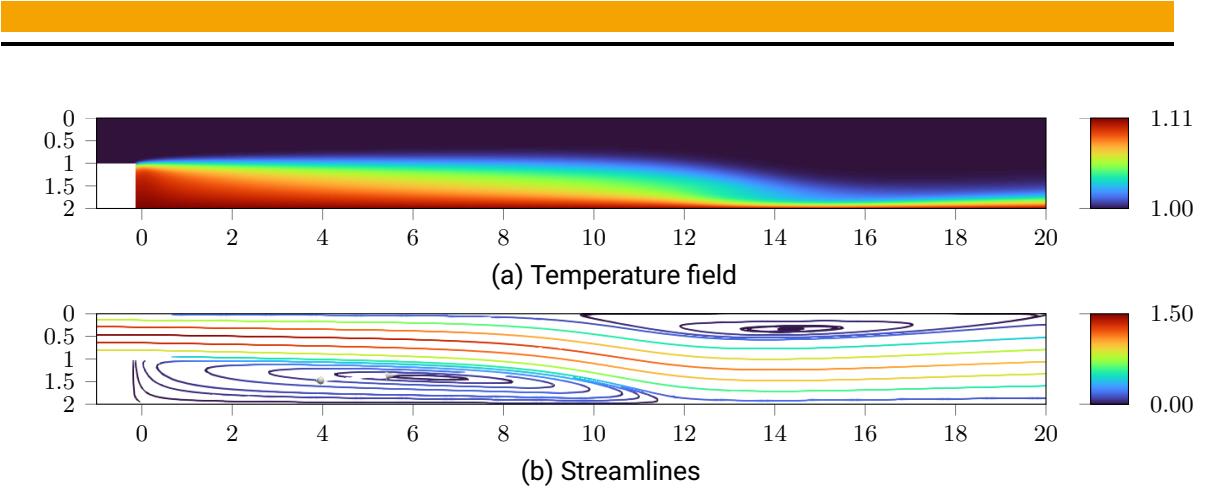


Figure 4.8: Temperature profile and streamlines corresponding to the backward-facing Step configuration for $\text{Re} = 400$ and an expansion ratio of two.

2016 is solved. The fluid entering the system has a temperature equal to $\hat{T}_0 = 283 \text{ K}$ and the bottom wall is set to a constant temperature of $\hat{T}_1 = 313 \text{ K}$. The inlet temperature is used as the reference temperature, obtaining $T_0 = 1.0$ and $T_1 = 1.106$. In the work of Xie and Xi, 2016 results are reported for the local Nusselt numbers and the local friction coefficients f_d along the bottom wall ($y = 0$) for different expansion ratios and Reynolds numbers. By combining the definition of the Nusselt number ($\text{Nu} = \hat{h}\hat{L}/\hat{\lambda}$), Newton's law of cooling ($\hat{\mathbf{q}} = \hat{h}(\hat{T}_0 - \hat{T}_1)$), and Fourier's law of heat conduction ($\hat{\mathbf{q}} = \hat{\lambda}\hat{\nabla}\hat{T}$) a expression for the local Nusselt number is obtained.

$$\text{Nu}_{\text{loc}} = \frac{\hat{L}}{\hat{T}_0 - \hat{T}_1} \hat{\nabla}\hat{T} \cdot \hat{\mathbf{n}} \quad (4.3)$$

where \hat{L} is the reference length. $\hat{L} = \hat{S}$ is chosen to be consistent with the definition of the Reynolds number of the reference. Furthermore, the local friction factor can be written as

$$f_d = \frac{8\hat{\nu}}{(\hat{U}_{\text{mean}})^2} \hat{\nabla}\hat{u} \cdot \hat{\mathbf{n}} \quad (4.4)$$

Simulations were conducted for different Reynolds numbers and expansion ratios. In Figure 4.8 the temperature field and the streamlines corresponding to a calculation with $\text{Re} = 700$ are shown. Here, the apparition of the secondary vortex is seen in the top wall. Note that only a small part of the computational domain is shown. Far away from the step, a lightly skewed parabolic velocity profile is obtained, which is influenced by the density variations on the vertical direction.

For this range of temperature differences, the temperature profile is just influenced by conductive effects, since no appreciable natural convection phenomena appears. For larger temperature differences, Rayleigh-Bénard type instabilities would appear in the flow. This type of system will be treated later in Section 4.2.5.

It should be noted here that the results obtained using the XNSEC-solver are substantially different from those reported by Xie and Xi, 2016, and will not be shown here. However, in the work of Hennink, 2022 the same is also reported, stating that with his method it was not possible to reproduce the results presented by Xie and Xi, 2016.

In Figure 4.9 the local friction factor and local Nusselt number along the wall $y = 0$ are plotted for $\text{Re} = 700$ and $\text{ER} = 2$. Comparing the results from the XNSEC-solver with those

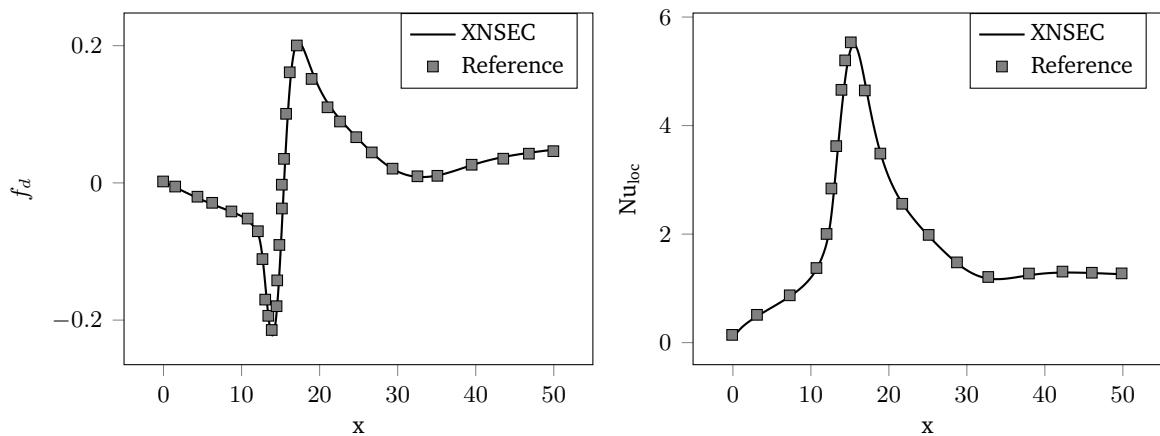


Figure 4.9: Local friction factor and local Nusselt number along the bottom wall of the backward-facing step for $\text{Re} = 700$ and an expansion ratio of two. The solid lines corresponds to our solution and the marks to the reference (Hennink, 2022)

reported in Hennink, 2022 a very good agreement can be observed. With this test it is possible to confirm that the XNSEC solver is able to deal with complex systems where heat transfer is present. However, for the range of temperature differences involved in this case, the variation of physical parameters such as density, viscosity and thermal conductivity with respect to temperature has no appreciable influence on the simulated flow fields. The next two test-cases will show how the XNSEC-solver is able to simulate low-Mach number flows with a considerable temperature difference.

4.2.2 Couette flow with vertical temperature gradient

As a further test case for the low-Mach solver, a Couette flow with a vertical temperature gradient is considered. This configuration was already studied in Klein et al., 2016, where the SIMPLE algorithm was used in an DG framework for the solution of the governing equations. In this section, the results from said publication are reproduced by using the XNSEC-solver, which features a fully coupled algorithm, in contrast to the SIMPLE solver, which solves the system in a segregated way. Additionally, it will be shown how the implemented solver performs in relation to the SIMPLE based solver in terms of runtime.

Set-up

In Figure 4.10 a schematic representation of the test case is shown. The domain is chosen as $\Omega = [0, 1] \times [0, 1]$, and Dirichlet boundary conditions are used for all boundaries. The upper wall corresponds to a moving wall ($u = 1$) with a fixed temperature $T = T_h$. The bottom wall is static ($u = 0$) and has a constant temperature $T = T_c$. Additionally, the system is subjected to a gravitational field, where the gravity vector only has a component in the y direction. Under these conditions, the x -component of velocity, pressure, and temperature are only dependent on the y coordinate, that is, $u = u(y)$, $T = T(y)$ and $p = p(y)$. The governing equations

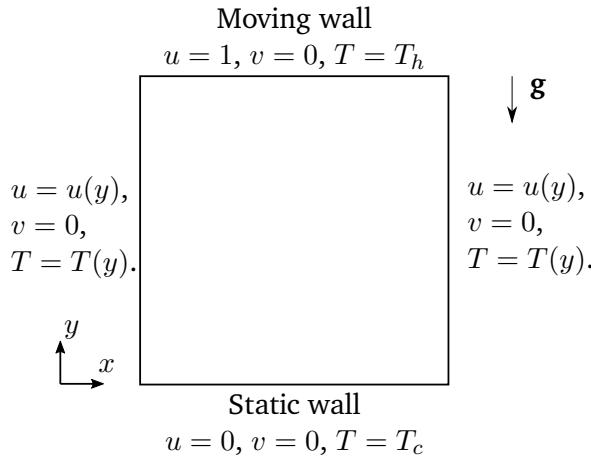


Figure 4.10: Schematic representation of the Couette flow with temperature difference test case.

(Equation (2.1)) reduce to

$$\frac{1}{\text{Re}} \frac{\partial}{\partial y} \left(\mu \frac{\partial u}{\partial y} \right) = 0, \quad (4.5a)$$

$$\frac{\partial p}{\partial y} = -\frac{\rho}{\text{Fr}^2}, \quad (4.5b)$$

$$\frac{1}{\text{Re} \text{Pr}} \frac{\partial}{\partial y} \left(\lambda \frac{\partial T}{\partial y} \right) = 0. \quad (4.5c)$$

By assuming a temperature dependence of the transport properties according to a Power Law ($\mu = \lambda = T^{2/3}$) it is possible to find an analytical solution for this problem.

$$u(y) = C_1 + C_2 \left(y + \frac{T_c^{5/3}}{T_h^{5/3} - T_c^{5/3}} \right)^{3/5}, \quad (4.6a)$$

$$p(y) = -\frac{5p_0}{2\text{Fr}^2} \frac{\left(y \left(T_h^{5/3} - T_c^{5/3} \right) + T_c^{5/3} \right)^{2/5}}{\left(T_h^{5/3} - T_c^{5/3} \right)} + C, \quad (4.6b)$$

$$T(y) = \left(C_3 - \frac{5}{3} C_4 y \right)^{3/5}. \quad (4.6c)$$

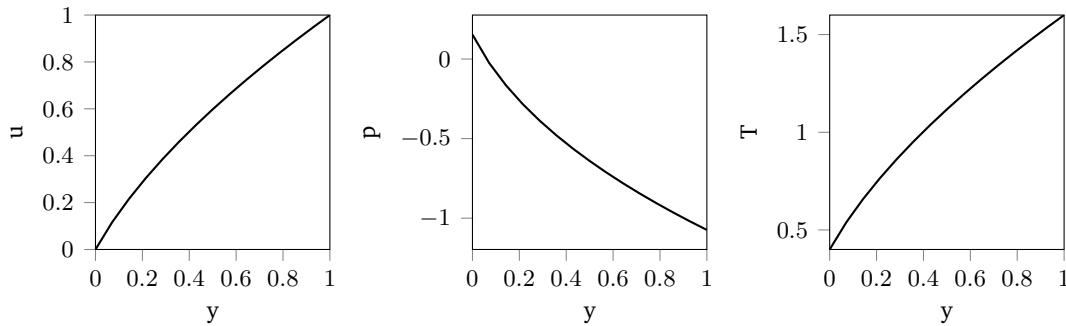


Figure 4.11: Solution of the Couette flow with vertical temperature gradient using a Power-Law.

Where the constants C_1 , C_2 , C_3 and C_4 are determined using the boundary conditions on the upper and lower walls and are given by

$$C_1 = \frac{\left(\frac{T_c^{5/3}}{T_h^{5/3} - T_c^{5/3}}\right)^{3/5}}{\left(\frac{T_c^{5/3}}{T_h^{5/3} - T_c^{5/3}}\right)^{3/5} - \left(\frac{T_h^{5/3}}{T_h^{5/3} - T_c^{5/3}}\right)^{3/5}} \quad (4.7a)$$

$$C_2 = \frac{1}{\left(\frac{T_h^{5/3}}{T_h^{5/3} - T_c^{5/3}}\right)^{3/5} - \left(\frac{T_c^{5/3}}{T_h^{5/3} - T_c^{5/3}}\right)^{3/5}} \quad (4.7b)$$

$$C_3 = T_c^{5/3}, \quad (4.7c)$$

$$C_4 = \frac{3}{5} \left(T_c^{5/3} - T_h^{5/3} \right) \quad (4.7d)$$

and C is a real-valued constant determined by an arbitrary zero level for the pressure. The dimensionless parameters are set as $\text{Re} = 10$ and $\text{Pr} = 0.71$, $T_h = 1.6$, and $T_c = 0.4$ for all calculations. The system is considered open and $p_0 = 1.0$. The Froude number is calculated as

$$\text{Fr} = \left(\frac{2\text{Pr}(T_h - T_c)}{(T_h + T_c)} \right)^{1/2}. \quad (4.8)$$

A derivation for Equation (4.8) will be given in Section 4.2.3. In Figure 4.11 the solutions for the velocity, pressure and temperature are shown. The results are for a mesh with 26×26 elements and a polynomial degree of three for u and T , and a polynomial degree of two for p . The vertical velocity v is zero everywhere.

h-convergence study

The convergence properties of the DG method for this nonisothermal system were studied using the analytical solution described before. The domain is discretized and solved in uniform Cartesian meshes with 16×16 , 32×32 , 64×64 and 128×128 elements. The polynomial degrees for the velocity and temperature are changed from one to four and for the pressure from zero to three. The convergence criterion described in Section 3.2.2 was used for all calculations. The analytical solutions given by Equation (4.6) are used as Dirichlet boundary conditions on

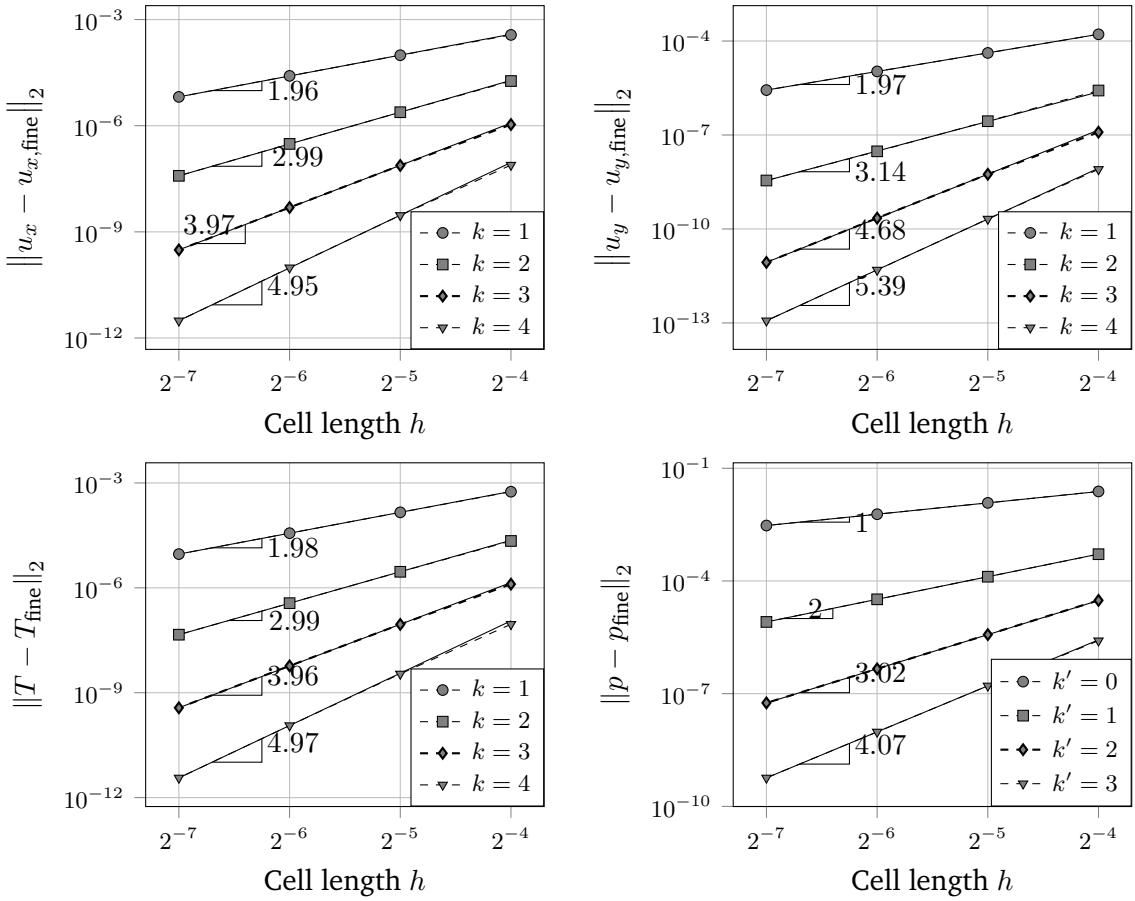


Figure 4.12: Convergence study of the Couette-flow with temperature difference. A power-law is used for the transport parameters.

all the boundaries of the domain. The global error is calculated against the analytical solution using a L^2 norm. In Figure 4.12 the results of the h-convergence study are shown. Recall that, for increasing polynomial order, the expected order of convergence is given by the slope of the line curve when cell length and errors are presented in a log-log plot. Due to the mixed-order formulation used, the slopes should be equal to k for the pressure and equal to $k + 1$ for all other variables. It is observed that the expected convergence rates are reached for all variables.

Comparison with SIMPLE

As mentioned before, a solver for solving low-Mach number flows based on the SIMPLE algorithm (presented in Klein et al., 2016) has already been developed and implemented within the BoSSS framework. Although the solver was validated and shown to be useful for a wide variety of test cases, there were also disadvantages inherent to the SIMPLE algorithm. For example, within the solution algorithm, Picard-type iterations are used to search for a solution. This usually requires some prior knowledge from the user in order to select suitable relaxation factor values that provide stability to the algorithm, but at the same time do not slow down the computation substantially. The intention of this subsection is to show a comparison of

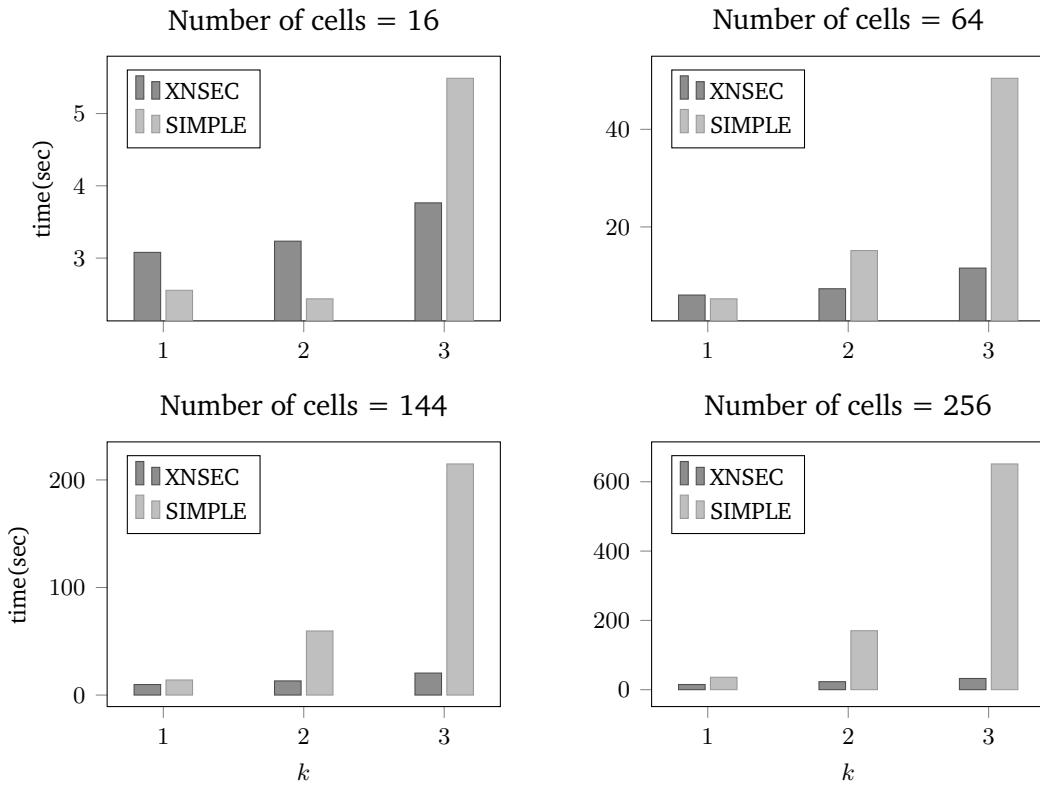


Figure 4.13: Runtime comparison of the DG-SIMPLE solver and the XNSEC-solver for the Couette flow with vertical temperature gradient for different polynomial degrees k and number of cells.

runtimes of the calculation of the Couette flow with vertical temperature gradient between the DG-SIMPLE algorithm (Klein et al., 2016) and the XNSEC-solver. Calculations were performed on uniform Cartesian meshes with 16×16 , 32×32 , 64×64 and 128×128 elements, and with varying polynomial degrees between one and three for the velocity and temperature, and between zero and two for the pressure. All calculations were initialized with a zero velocity and pressure field, and with a temperature equal to one in the whole domain. The calculations were performed single-core and the convergence criteria is set to 10^{-8} for both solvers. The under-relaxation factors for the SIMPLE algorithm were set for all calculations to 0.8, 0.5 and 1.0 for the velocity, pressure and temperature, respectively.

In figure Figure 4.13 a comparison of the runtimes from both solvers is shown. It is clearly appreciated how the runtimes of the SIMPLE algorithm are higher for almost all of the cases studied. Obviously the under-relaxation parameters of the SIMPLE algorithm have an influence on the calculation times and an appropriate selection of them could decrease the runtimes. This is a clear disadvantage because the selection of adequate factors is highly problem dependent and requires some previous expertise from the user. On the other hand, the globalized Newton method used by the XNSEC-solver avoid this problem by using a more sophisticated method and heuristics in order to find a better path to the solution.

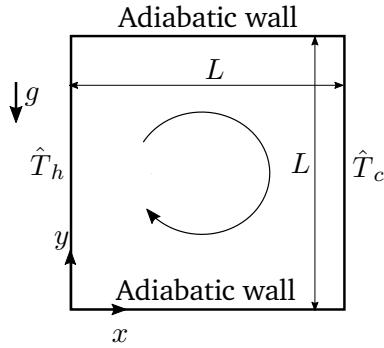


Figure 4.14: Schematic representation of the differentially heated cavity problem.

4.2.3 Differentially heated cavity problem

The differentially heated cavity problem is a classical benchmark case that is often used to assess the ability of numerical codes to simulate variable density flows (Pailiere et al., 2000; Vierendeels et al., 2003; Tyliszczak, 2014). The test case has the particularity that deals with a closed system, where the thermodynamic pressure p_0 is a parameter that must be adjusted so that the mass is conserved. The thermodynamic pressure p_0 determines the density field, which in turn appears in the momentum equation and the energy equation, making it necessary to use an adequate algorithm to solve the system. This point presents a special difficulty for the solution, since the calculation of p_0 requires knowledge of the temperature field on the whole computational domain, inducing a global coupling of the variables.

The system is a fully enclosed two-dimensional square cavity filled with fluid. A sketch of the problem is shown in Figure 4.14. The left and right walls of the cavity have constant temperatures \hat{T}_h and \hat{T}_c , respectively, with $\hat{T}_h > \hat{T}_c$, and the top and bottom walls are adiabatic. A gravity field induces fluid movement because of density differences caused by the difference in temperature between the hot and cold walls. The natural convection phenomenon is characterized by the Rayleigh number, defined as

$$\text{Ra} = \text{Pr} \frac{\hat{g} \hat{\rho}_{\text{ref}}^2 (\hat{T}_h - \hat{T}_c) \hat{L}_{\text{ref}}^3}{\hat{T}_{\text{ref}} \hat{\mu}_{\text{ref}}^2}, \quad (4.9)$$

For small values of Ra, conduction dominates the heat transfer process, and a boundary layer covers the entire domain. On the other hand, large values of Ra represent a flow dominated by convection. When the number Ra increases, a thinner boundary layer is formed. Following Vierendeels et al., 2003, a reference velocity for buoyancy-driven flows can be defined as

$$\hat{u}_{\text{ref}} = \frac{\sqrt{\text{Ra}} \hat{\mu}_{\text{ref}}}{\hat{\rho}_{\text{ref}} \hat{L}_{\text{ref}}}. \quad (4.10)$$

The Rayleigh number is then related to the Reynolds number according to

$$\text{Re} = \sqrt{\text{Ra}}. \quad (4.11)$$

Thus, it is sufficient to select a Re number in the simulation, fixing the value of the Ra number. The driving temperature difference ($\hat{T}_h - \hat{T}_c$) appearing in Equation (4.9) can be represented

as a non-dimensional parameter:

$$\varepsilon = \frac{\hat{T}_h - \hat{T}_c}{2\hat{T}_{\text{ref}}}. \quad (4.12)$$

Using these definitions, the Froude number can be calculated as

$$Fr = \sqrt{\text{Pr}2\varepsilon}. \quad (4.13)$$

The results of the XNSEC solver are compared with those of the reference solution for $\hat{T}_{\text{ref}} = 600\text{K}$ and $\varepsilon = 0.6$. All calculations assume a constant Prandtl number equal to 0.71. The dependence of viscosity and heat conductivity on temperature is calculated using Sutherland's law (Equation (2.29)). The non-dimensional length of the cavity is $L = 1$. The non-dimensional temperatures T_h and T_c are set to 1.6 and 0.4, respectively. The non-dimensional equation of state (Equation (2.26)) depends only on the temperature and reduces to

$$\rho = \frac{p_0}{T}. \quad (4.14)$$

The thermodynamic pressure p_0 in a closed system must be adjusted to ensure mass conservation. For a closed system is given by

$$p_0 = \frac{\int_{\Omega} \rho_0 dV}{\int_{\Omega} \frac{1}{T} dV} = \frac{m_0}{\int_{\Omega} \frac{1}{T} dV}, \quad (4.15)$$

where Ω represents the complete closed domain. The initial mass of the system m_0 is constant and is set $m_0 = 1.0$. Note that the thermodynamic pressure is a parameter with a dependence on the temperature of the entire domain. This makes necessary the use of an iterative solution algorithm, so that the solution obtained respects the conservation of mass. Within the solution algorithm of the XNSEC-solver, Equation (4.15) is used to update the value of the thermodynamic pressure after each Newton iteration. The average Nusselt number is defined for a given wall Γ as

$$\text{Nu}_{\Gamma} = \frac{1}{T_h - T_c} \int_{\Gamma} k \frac{\partial T}{\partial x} dy. \quad (4.16)$$

Comparison of results with the benchmark solution

Here a comparison of the results obtained with the XNSEC-solver and the results presented in the work of Vierendeels et al., 2003 is made. They solved the fully compressible Navier-Stokes equations on a stretched grid with 1024×1024 using a finite-volume method with quadratic convergence, providing very accurate results that can be used as reference. The benchmark results are presented for $\text{Ra} = \{10^2, 10^3, 10^4, 10^5, 10^6, 10^7\}$. In this range of Rayleigh numbers, the problem has a steady-state solution. The cavity is represented by the domain $[0, 1] \times [0, 1]$. For all calculations in this subsection, the simulations are done with a polynomial degree of four for both velocity components and temperature and three for the pressure. The mesh is in an equidistant 128×128 mesh.

Preliminary calculations showed that for cases up to $\text{Ra} = 10^5$ the solution of the system using Newton's method presented in Section 3.2.1 is possible without further modifications, while for higher values the algorithm couldn't find a solution and stagnates after certain number of iterations. The homotopy strategy mentioned in Section 3.2 is used to overcome this problem and obtain solutions for higher Rayleigh numbers. Here, the Reynolds number is selected as the homotopy parameter and continuously increased until the desired value is reached.

In Figures 4.16 to 4.18 the temperature and velocity profiles across the cavity for different Rayleigh numbers are shown. The profiles calculated with the XNSEC-solver agree closely to the benchmark solution. As expected, an increase of the acceleration of the fluid in the vicinity of the walls for increasing Rayleigh numbers is observed.

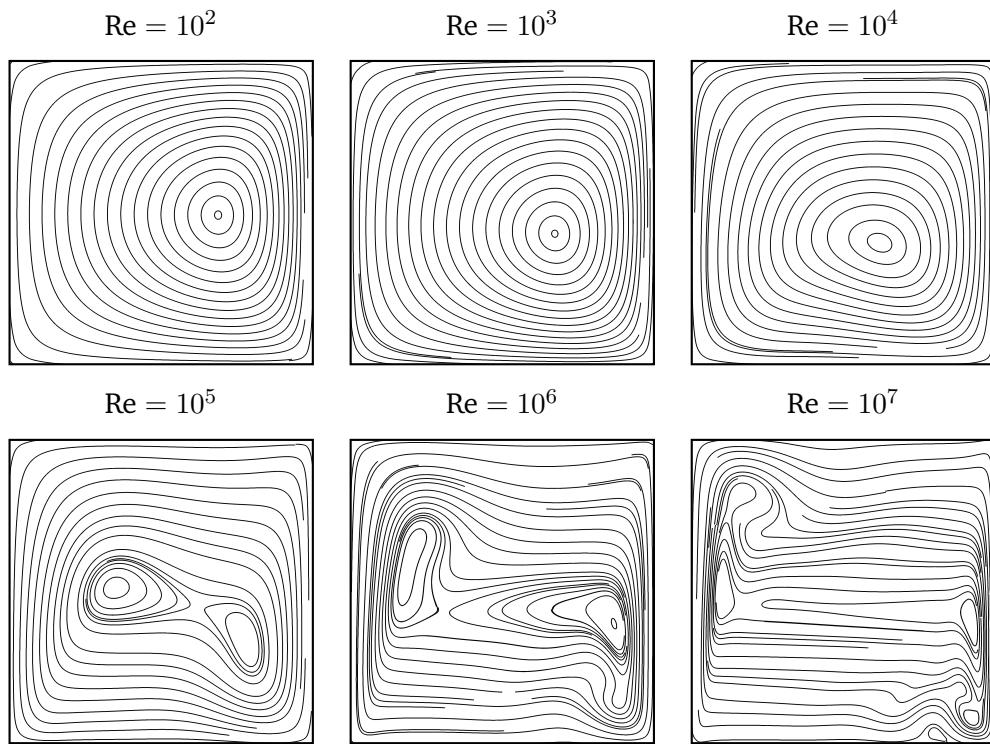


Figure 4.15: Streamlines of the heated cavity configuration with $\epsilon = 0.6$ for different Reynold numbers.

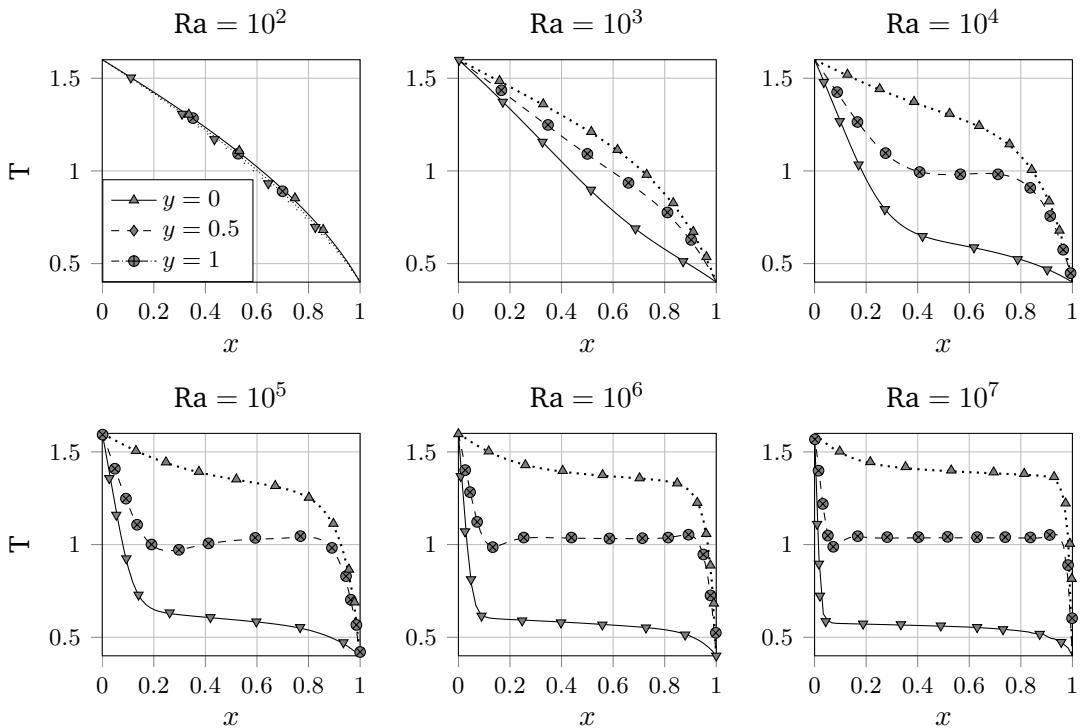


Figure 4.16: Temperature profiles for the differentially heated square cavity along different vertical levels. Solid lines represent the XNSEC-solver solution and marks the benchmark solution.

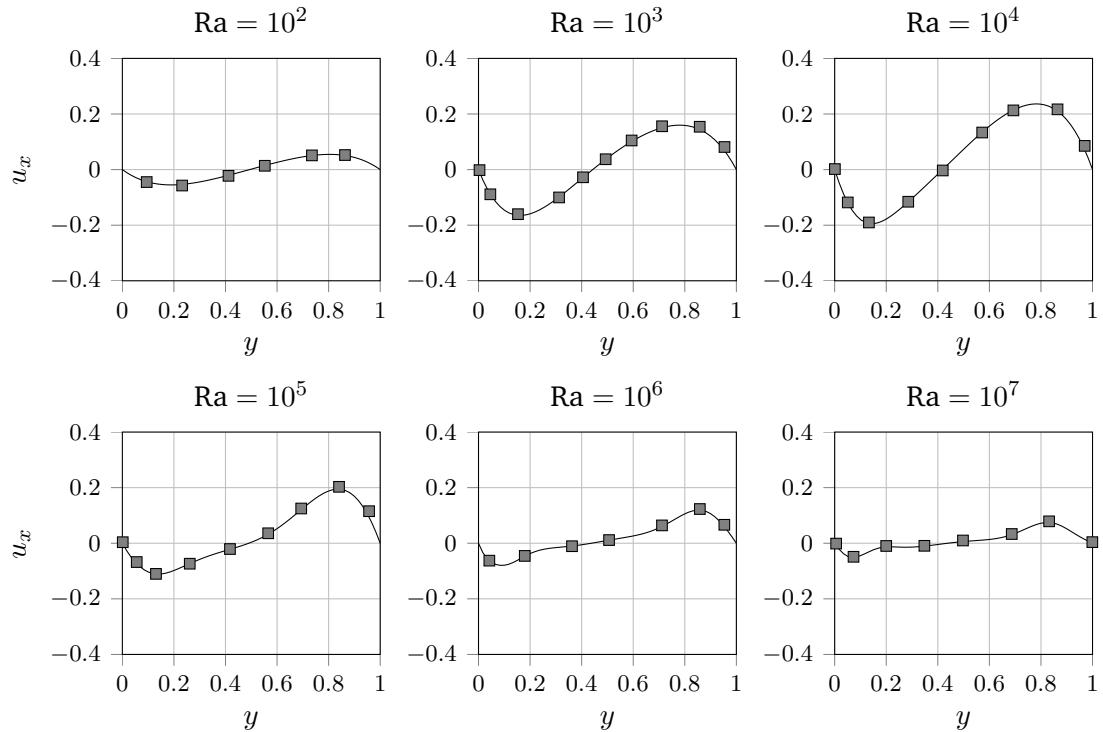


Figure 4.17: Profiles of the x-velocity component for the differentially heated square cavity along the vertical line $x = 0.5$. Solid lines represent the XNSEC-solver solution and marks the benchmark solution.

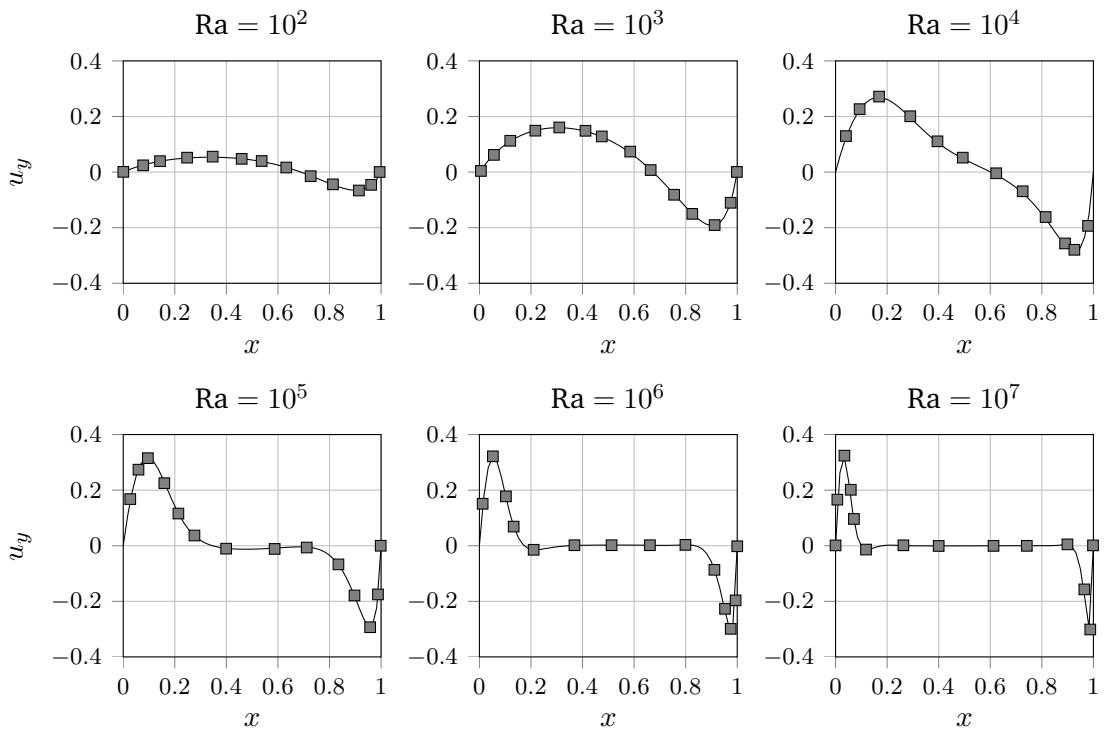


Figure 4.18: Profiles of the y-velocity component for the differentially heated square cavity along the horizontal line $y = 0.5$. Solid lines represents the XNSEC-solver solution and marks the benchmark solution.

Rayleigh	p_0	$p_{0,\text{ref}}$	Nu_h	Nu_c	Nu_{ref}
10^2	0.9574	0.9573	0.9787	0.9787	0.9787
10^3	0.9381	0.9381	1.1077	1.1077	1.1077
10^4	0.9146	0.9146	2.2180	2.2174	2.2180
10^5	0.9220	0.9220	4.4801	4.4796	4.4800
10^6	0.9245	0.9245	8.6866	8.6791	8.6870
10^7	0.9225	0.9226	16.2411	16.1700	16.2400

Table 4.2: Comparison of calculated Nusselt numbers of the hot and cold wall and Thermodynamic pressure p_0 reported values by Vierendeels et al., 2003 for the differentially heated cavity.

A comparison of the thermodynamic pressure and the Nusselt numbers to the benchmark solution was also made. The results are shown in Table 4.2. The thermodynamic pressure is obtained from Equation (4.15), and the average Nusselt number is calculated with Equation (4.16). The results obtained with the XNSEC-solver agree very well with the reference results, as can be seen for the thermodynamic pressure, which differs at most in the fourth decimal place. Note that the average Nusselt number of the heated wall (Nu_h) and the Nusselt number of the cold wall (Nu_c) are different. As the Rayleigh number grows, this discrepancy becomes larger, hinting that, at such Rayleigh numbers, the mesh used is not refined enough to adequately represent the thin boundary layer and more complex flow structures appearing in high-Rayleigh number cases. While for an energy conservative system Nu_h and Nu_c should be equal, for the DG-formulation this is not the case, since conservation is only ensured locally and the global values can differ. This discrepancy can be seen as a measure of the discretization error of the DG formulation and should decrease as the mesh resolution increases. This point will be discussed in the next section.

Convergence study

An h -convergence study of the XNSEC solver was conducted using the heated cavity configuration. Calculations were performed for polynomial degrees $k = 1, 2, 3, 4$ and equidistant regular meshes with, respectively, 8×8 , 16×16 , 32×32 , 64×64 , 128×128 and 256×256 elements. The L^2 -Norm was used to calculate errors against the solution in the finest mesh. The results of the h -convergence study for varying polynomial orders k are shown in Figure 4.19. It is observed how the convergence rates scale approximately as $k + 1$. Interestingly, for $k = 2$ the rates are higher than expected. On the other hand, some degeneration is observed in convergence rates for $k = 4$. This strange behavior can be explained if one considers that the heated cavity presents a singular behavior at the corners -similar to the problem previously exposed for the lid-driven cavity -, which causes global pollution in the convergence behavior of the algorithm.

As discussed in the previous section, the difference in the average values of the Nusselt number on the hot wall Nu_h and the cold wall Nu_c is a direct consequence of the spatial discretization error and should decrease for finer meshes. In Figure 4.20 the convergence behavior of the Nusselt number is presented for different polynomial degrees k , different number of elements and for two different Ra numbers. As expected, it can be observed that this discrepancy is smaller when a larger number of elements is used. It can also be seen that Nu_h reaches the expected solution of cells for a much smaller number of elements. This can

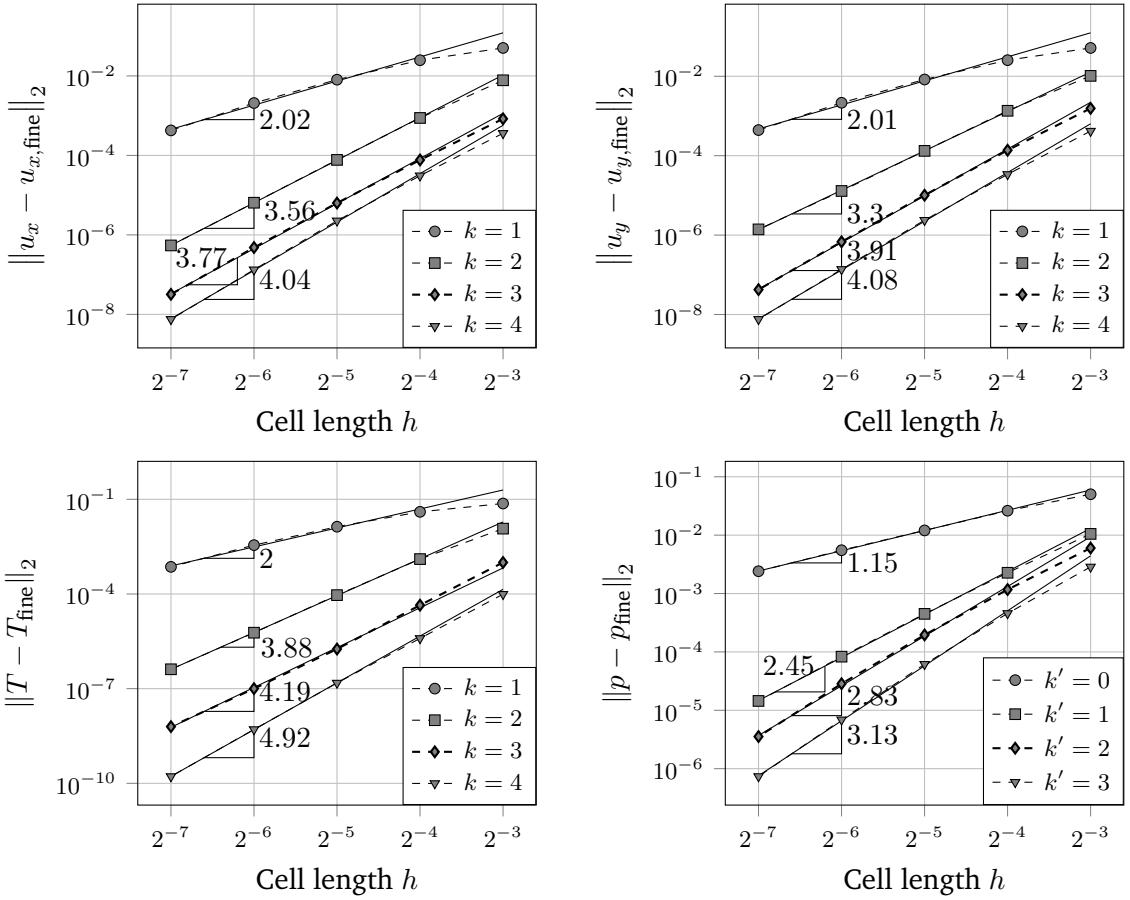


Figure 4.19: Convergence study of the differentially heated cavity problem for $\text{Ra} = 10^3$.

be explained if one thinks that more complex phenomena take place near the cold wall (see Figure 4.15), which makes necessary a finer mesh resolution in that area.

The results presented in this section allow us to conclude that the implemented solver is capable of dealing with flows with variable densities, and in particular in closed spaces. Additionally, it was observed that even for this complex test, convergence properties close to those expected from the DG-method are obtained. In this section only systems with a steady state solution were treated. In the next section the ability of the solver to compute flows with varying densities in non-steady state will be shown.

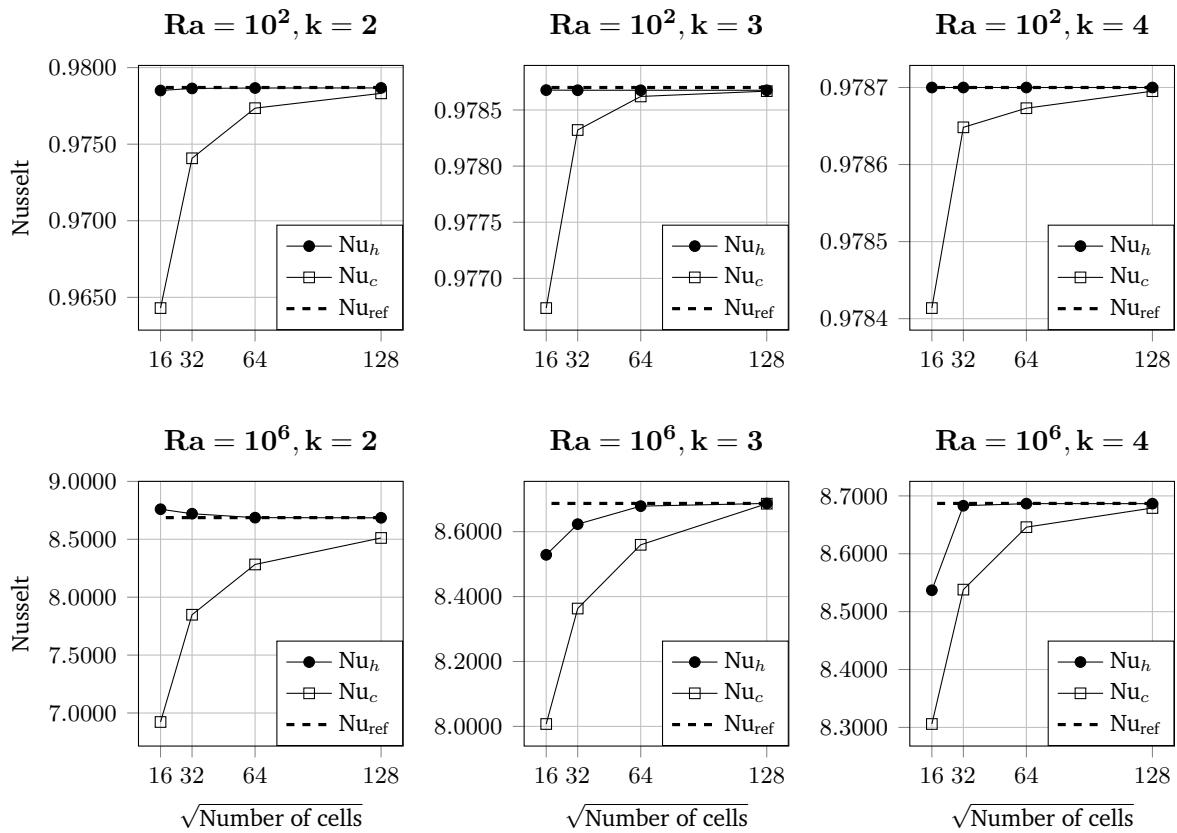


Figure 4.20: Nusselt numbers of the differentially heated square cavity at the hot wall (Nu_h) and the cold wall (Nu_c) for different number of cells and polynomial order k . The reference values from Vierendeels et al., 2003 are shown with dashed lines.

Influence of the penalty factor

A point not still discussed is the choice of the safety parameter μ_0 of the penalty terms from the SIP discretization. Table X shows results obtained for $\text{Ra} = 10^3$, for different polynomial degrees and penalty safety factor. For the tests presented here, the penalty terms of the difussive terms from the momentum and energy equations are considered equal. Furthermore, the number of elements in the mesh is selected in such a way that the number of degrees of freedom remains approximately constant for each simulation.

It is possible to see that the penalty safety factor (and therefore the penalty term) can have a great influence on the solution. If the value chosen is very small, as in the case of the table for $\mu = 0.01$, the algorithm is not able to find a solution. On the other hand, if the chosen value is too high, the error also increases. It can be concluded that an optimal value for the penalty factor exists.

It is also noticeable that, maintaining a constant penalty safety factor, increasing the polynomial degree for an approximately constant number of dofs gives an improvement in the results compared to the literature. Although for this testcase the effect of the penalty factor on the solution is not very large, the effect could be considerable, especially when dealing with more complex geometries and coarser meshes. The value $\mu_0 = 4$ has shown to be a value that gives

μ	DofS	k	Nu_c	$\frac{Nu_c - Nu_{c,ref}}{Nu_{c,ref}} \times 10^2$	p_0	$\frac{p_0 - p_{0,ref}}{p_{0,ref}} \times 10^4$
0.01	2	6804	0.549483*	50.39424	0.899757*	408.7292
	3	7056	0.722593*	34.76637	0.936085*	21.48436
	4	6655	-0.50954*	146	1.016691*	837.7683
1	2	6804	1.090047	1.593667	0.938192	0.980674
	3	7056	1.102072	0.508037	0.938057	0.453674
	4	6655	1.105225	0.22348	0.938046	0.570494
4	2	6804	1.089332	1.65817	0.93843	3.521926
	3	7056	1.102261	0.491027	0.938076	0.25384
	4	6655	1.105359	0.211372	0.938047	0.561709
16	2	6804	1.08694	1.874166	0.939109	10.75641
	3	7056	1.102266	0.490563	0.938124	0.251627
	4	6655	1.105439	0.204153	0.93805	0.537265

Table 4.3: Thermodynamic pressure and cold-side Nusselt number for different penalty safety factors in a heated cavity with $Ra = 10^3$. Values marked with an asterisk are from problems not converged after 100 iterations.

stability to the scheme and is used for all simulations in this thesis, as already has been done in many works (Krause and Kummer, 2017; Kummer, 2017; Smuda, 2021).

4.2.4 Flow over a circular cylinder

A further thest case of the XNSEC solver is the simulation of flow over a circular cylinder. The results shown section are based on the work by Miao, 2022

The simulation of a 2D flow over an obstacle exhibits different flows states depending on the Reynolds number. For low Reynolds numbers, the flow is laminar and stationary. When the Reynolds number reaches a critical value, the flow becomes non-stationary and eventually turbulent. In particular, for $50 \leq Re \leq 160$ the behavior of the fluid is laminar with an unstationary periodic character, and the well-known vortex shedding phenomenon appears (Sharma and Eswaran, 2004). In this section the ability of the XNSEC-solver for dealing with isothermal and non-isothermal unsteady flow will be assesed. THis is done by calculating the Strouhal number, average drag and lift coefficients and the Nusselt number and comparing them to reference solutions.

Set-up

Figure 4.21 shows the geometry of the problem. In the center of the domain is located a heated cylinder of diameter $d = 1$, which is subjected to a flow of constant velocity magnitude. The size of the computational domain is chosen as $D = 59d$, which is large enough so that the outlet boundary conditions do not influence the solution. The left half of the boundaries of the computational domain corresponds to a velocity inlet with constant velocity $(u, v) = (1, 0)$ and temperature $T = T_\infty$. The right half of the domain corresponds to a pressure outlet. The boundary condition corresponding to the heated cylinder is a no-slip wall $((u, v) = (0, 0))$, with a constant temperature $T = T_h$. The system is an open system, and the thermodynamic pressure has a constant value set to $p_0 = 1$.

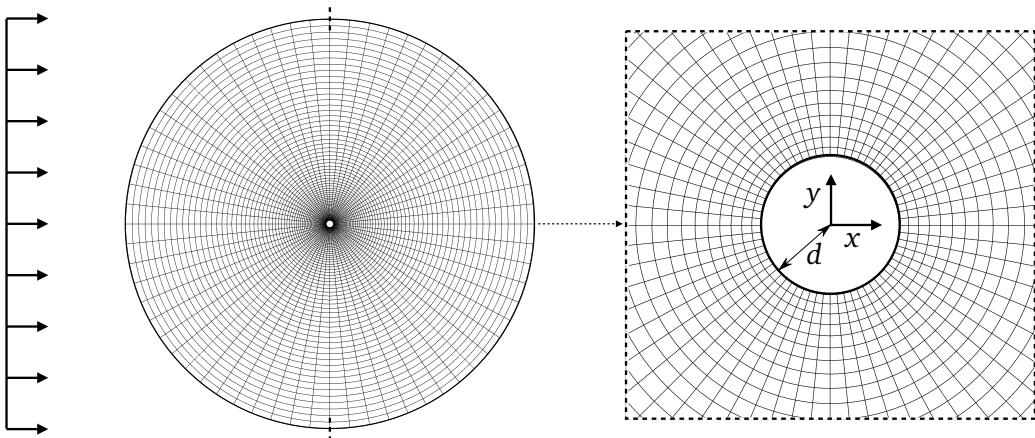


Figure 4.21: Schematic representation of the heated circular cylinder.

As mentioned, a isothermal and non-isothermal system is considered in this section. A reference temperature of $\hat{T}_{\text{ref}} = 298.15 \text{ K}$ is selected. The conditions for the velocity inlet are for the isothermal case a dimensionless temperature of $T_h = 1.0$ and $T_\infty = 1$, while for the non-isothermal $T_h = 1.5$ and $T_\infty = 1.0$. A Reynolds number of 100 is used, for which the flow is known to be unsteady and periodic. Gravity effects are taken as negligible. The prandtl number has a constant value of $\text{Pr} = 0.71$ and the heat capacity ratio $\gamma = 1.4$. The transport parameters are calculated with Sutherlands law which is given by Equation (2.29) and the equation of state for the density is Equation (2.26).

For all calculations a polynomial degree of order three is used for both velocity components and the temperature, and two for pressure. In this simulation a curved mesh consisting of 64 elements in the radial direction and 64 elements in the angular direction is used. The use of a curved mesh for this problem was done primarily to adequately represent the geometry of the heated cylinder. Another possibility could have been to use a method such as a Immersed Boundary Method (which is also possible to do in the BoSSS-framework), but it is beyond the scope of this work.

One point to note regarding the use of curved meshes within the DG-method (and in all High-order methods), is that special care has to be taken in the representation of curved elements in order to use correctly quadrature rules (Bassi and Rebay, 1997). This is critical to preserve the convergence properties of DG-methods. In particular, since the highest degree of the polynomials used in this simulation is three, elements of the bi-cubic type are used, where 16 nodes are used per element for the discretization for a two-dimensional element. Furthermore, the time discretization is performed with a BDF-3 scheme, and the time derivative of the continuity equation is calculated with a second order backward difference scheme (see Section 3.1.3). The simulation time corresponds to $t = 100$, and constant timesteps of $\Delta t = 0.2$ are used. The initial conditions are

$$u(t=0) = 1 + u^{\text{vortex}}, \quad (4.17a)$$

$$v(t=0) = 0 + v^{\text{vortex}}, \quad (4.17b)$$

$$T(t=0) = 1, \quad (4.17c)$$

$$p(t=0) = 0. \quad (4.17d)$$

Here, u^{vortex} and v^{vortex} are the velocity component of a vortex field of radius r , strength a and

central point (x^o, y^o) defined by

$$u^{\text{vortex}}(x, y) = \begin{cases} -a(y - y^o) & \text{if } \sqrt{(x - x^o)^2 + (y - y^o)^2} \leq r \\ 0 & \text{if } \sqrt{(x - x^o)^2 + (y - y^o)^2} > r \end{cases} \quad (4.18\text{a})$$

$$v^{\text{vortex}}(x, y) = \begin{cases} a(x - x^o) & \text{if } \sqrt{(x - x^o)^2 + (y - y^o)^2} \leq r \\ 0 & \text{if } \sqrt{(x - x^o)^2 + (y - y^o)^2} > r \end{cases} \quad (4.18\text{b})$$

The reason for placing a vortex in the initial conditions is to include a perturbation in the system that triggers the vortex shedding phenomenon. The vortex moves with the flow and is eventually advected from the calculation domain. Specifically, for this simulation, a vortex of radius $r = 1$ and strength $a = 1$ is placed at $(x^o, y^o) = (2, 0)$. It is worth mentioning that the inclusion of the vortex in the initial conditions is not imperative to make the vortex-shedding phenomenon emerge, but it is a way to accelerate its appearance. For the range of Reynolds numbers mentioned, even instabilities of the numerical method should be enough to cause the phenomenon to arise, but in a much slower way.

The variables lift coefficient C_L , drag coefficient C_D , Strouhal number St , and Nusselt number Nu are calculated and compared with reference results. These characteristic quantities are defined as

$$C_L = \frac{2F_L}{\rho_\infty u_\infty^2 d} \quad (4.19)$$

$$C_D = \frac{2F_D}{\rho_\infty u_\infty^2 d} \quad (4.20)$$

$$\text{St} = \frac{fd}{u_\infty} \quad (4.21)$$

$$\text{Nu} = \frac{d}{\Delta T} \frac{1}{\|\partial S\|_{\text{leb}}} \oint_{\partial S} \nabla T \cdot \mathbf{n} ds \quad (4.22)$$

F_L and F_D are the lift and drag force respectively, f is the vortex shedding frequency and $\|\text{leb}\| = \pi d$ is the circumference of the cylinder.

Isothermal case.

The isothermal case results are compared with the work of Sharma and Eswaran, 2004. They reported results for the case $\text{Re} = 100$ and $T_h = T_\infty$. The Strouhal number and average drag coefficient calculated with the XNSEC-solver are $\text{St} = 0.1639$ and $C_{D,\text{avg}} = 1.3103$, while the reference values $\text{St} = 0.164$ and $C_{D,\text{avg}} = 1.3183$, which means a error of less than a 0.6% on both quantities. Its worth noting that preliminar calculations with a implicit Euler scheme for the discretization of the temporal terms didnt cause the vortex shedding phenomenom to appear, making necesary a BDF-3 scheme.

Non-isothermal case.

A comparison of the calculation results for the non-isothermal case was performed based on the results reported in Shi et al., 2004, Wang et al., 2000 and Hennink, 2022. The temporal evolution of the characteristic quantities C_D , C_L and Nu is shown in Figure 4.22. The results agree very good with the references. The average Nusselt number is $\text{Nu} = 3.8434$, while

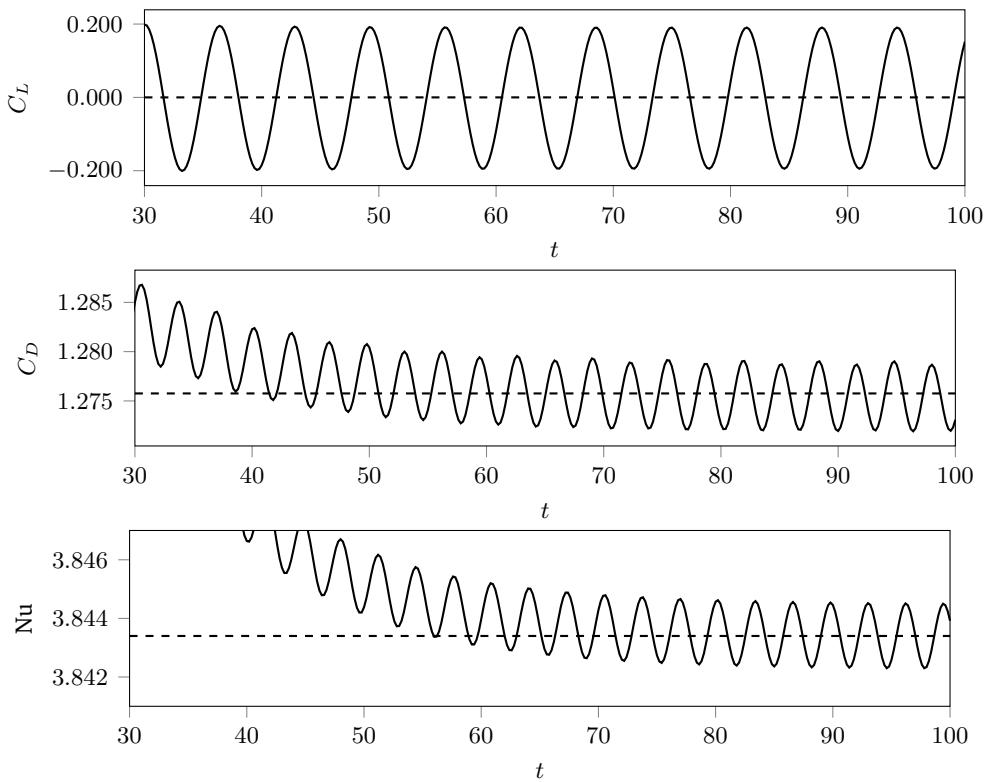


Figure 4.22: Temporal evolution of average Nusselt number, lift coefficient and drag coefficient of the heated cylinder

the reference value from Hennink, 2022 is $\text{Nu} = 3.804$, which corresponds to a difference of 1.04%. The Strouhal number is $\text{St} = 0.1538$ and the references report values of $\text{St} = 0.152$ and $\text{St} = 0.1536$, a difference of approximately 1%. It is possible then to conclude that the XNSEC-solver allows to simulate adequately unsteady non-isothermal flows, where the fluid properties do present a scalar dependence (in this case, on the temperature). It is important to note that the temperature variation in this test-case causes only a moderate variation in the density. As will be seen later, the temporal term appearing in the continuity equation is problematic in the case of larger density differences (Knijker, 2011), as it is a cause of numerical instabilities.

4.2.5 Rayleigh-Bénard Convection

The Rayleigh-Bénard convection is a configuration similar to the heated cavity (see Section 4.2.3) as the flow is also induced by buoyancy effects. The configuration consists of a fluid located between two horizontal plates maintained at different temperatures, with the lower temperature being higher than the upper temperature. It is known that under a certain Rayleigh number the flow presents a macroscopically stable behavior and the heat is simply transferred by conductive phenomena. When the Rayleigh number exceeds a certain critical value Ra_{crit} , the system becomes unstable, which causes a perturbation of the system to give rise to fluid motion, creating the so-called convection cells, also usually also referred to as Bénard cells.

In the following sections two aspects of this situation will be discussed by making use of

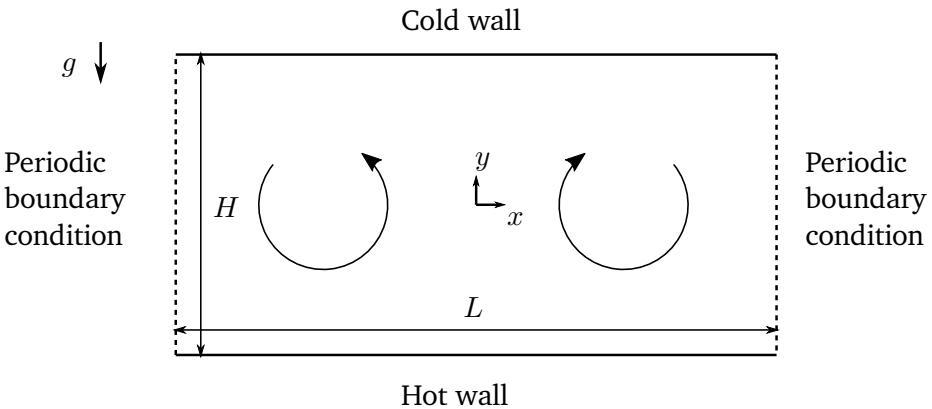


Figure 4.23: Geometry of the Rayleigh-Bénard convection problem. Convection rolls are sketched

different type of boundary conditions on the sides of the domain. First in Section 4.2.5 periodic boundary conditions are used, which allows to study a single pair of convection rolls and to calculate numerically the critical value Ra_{crit} , which is compared with theoretical values. Subsequently, in Section 4.2.5 a transient simulation of this configuration is performed by using pressure-outlet boundary conditions. The results shown section are based on the work by Miao, 2022

Periodic boundary conditions

In this section the fluid behavior will be analyzed by studying a system where a single convection-cell appears. Making use of the linear stability theory for the governing equations under the boussinesq assumption, it is possible to determine that for a system with rigid boundaries the critical Rayleigh number is $\text{Ra}_{\text{crit}} = 1707.762$ (Chandrasekhar, 1961). Moreover, the wave number is $a_c = 3.117$, which implies that the convective rolls develop at an aspect ratio of $2\pi/a_c = 2.016$. For the simulations presented in this section an aspect ratio of $L/H = 2$ is used, as is done by Kao and Yang, 2007. The geometry and boundary conditions of the analyzed problem can be found in Figure 4.23. The upper wall corresponds to a no-slip wall that is maintained at a constant temperature T_c . Similarly, the bottom wall is also a no-slip wall with a temperature T_h , with $T_h > T_c$. The boundary conditions on the left and right of the computational domain are periodic boundary conditions. Gravity has only one component in the negative direction of y .

For the range of Rayleigh numbers treated here, the simulations are steady state simulations. For all simulations in this section a regular Cartesian grid consisting of 32×64 cells, with dimensionless lengths $L = 2$ and $H = 1$ was used. The polynomial degree of both velocity components and temperature is four, and for pressure it is three. An open system is assumed, and $p_0 = 1.0$ throughout the simulation.

First, the stability of the XNSEC-solver will be studied by determining the critical value Ra_{crit} . As mentioned above, the theoretical value $\text{Ra}_{\text{crit}} = 1707.762$ was determined using the Boussinesq assumption in the governing equations, which, unlike the low mach equations, is only valid if the variation of temperature within the system is very small. For this reason, an analysis is performed for a dimensionless temperature difference $\epsilon = (T_h - T_c)/(T_h + T_c) = 0.0001$, meaning $T_h = 1.0001$ and $T_c = 0.9999$. The reference temperature is chosen as

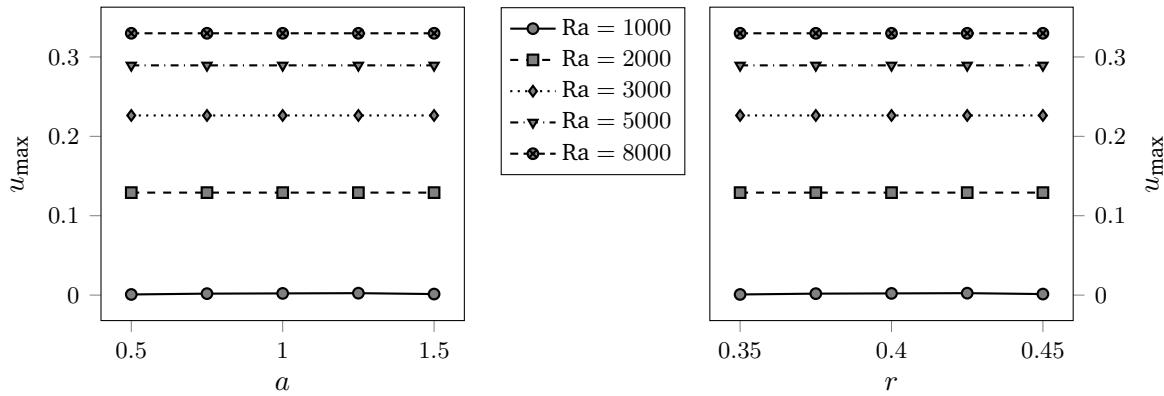


Figure 4.24: Maximum x-velocity in the Rayleigh-Bénard convection configuration for different a and r .

$\hat{T}_{\text{ref}} = 600 \text{ K}$. Since the XNSEC-solver is based on the low-Mach equations, this choice of low temperature difference allows to compare the present results with those obtained analytically using the Boussinesq approximation. The definition of the dimensionless numbers as well as the reference velocity are exactly the same as those mentioned in Section 4.2.3. The transport coefficients are calculated with Sutherlands Law.

Similarly to the case exposed in Section 4.2.4, velocity fields are initialized with vortices, which play the role within the simulation of a trigger for the inherent instabilities of the problem. In particular, two vortices with opposite directions of rotation are added. The velocity components of these are again given by equations Equation (4.18) and Equation (4.18). The coordinates of the first vortex are $(x^o, y^o) = (-0.5, 0)$ and it has a strength $a = 1$ and a radius $r = 0.4$. For the second vortex $(x^o, y^o) = (0.5, 0)$, $a = -1$ and $r = 0.4$. The initial conditions are

$$u(t=0) = 1 + u^{\text{vortex-left}} + u^{\text{vortex-right}}, \quad (4.23a)$$

$$v(t=0) = 0 + v^{\text{vortex-left}} + v^{\text{vortex-right}}, \quad (4.23b)$$

$$T(t=0) = 1, \quad (4.23c)$$

$$p(t=0) = -\frac{\rho y}{\text{Fr}^2}. \quad (4.23d)$$

It is worth noting that the initialization of the solver without the vortices leads the solver to a stationary solution where there is no fluid motion. Clearly, this is a solution of the equations, but, as already mentioned, it is an unstable solution.

First, a study was performed to demonstrate the independence of the steady-state solution from the chosen initial conditions. This is demonstrated in Figure 4.24, where for a given Rayleigh number the maximum velocity obtained inside the system is shown, varying the strength a or the radius r of the vortices. It is also apparent that the case $\text{Ra} = 1000$ does not exhibit a macroscopic fluid motion, while $\text{Ra} = 2000$ does. This points to the fact that the critical value is effectively in this range.

Subsequently, a series of simulations were performed with $a = 0.5$ y $r = 0.4$, and a bisection algorithm was used to find the critical Rayleigh value, obtaining $\text{Ra} = 1707.922$, as shown in Figure 4.25. Compared to the theoretical value $\text{Ra} = 1707.762$, it presents a difference of only 0.009%. In addition, the proportionality $u \propto \sqrt{\text{Ra} - \text{Ra}_{\text{Ra}}}$ that is expected by analytical arguments is also fulfilled, obtaining, in particular, $u_{\text{max}} = 0.008015\sqrt{\text{Ra} - 1707.922}$. It is possible

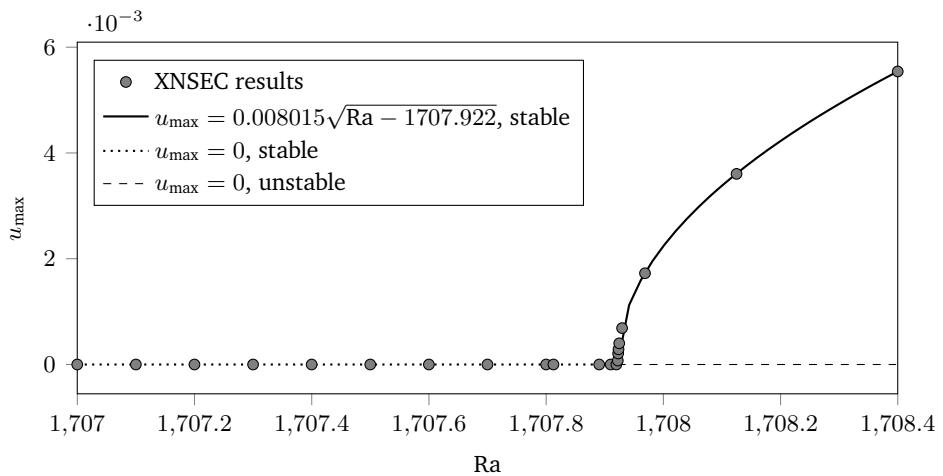


Figure 4.25: Stability behaviour of the Rayleigh-Bénard convection with $\epsilon = 0.0001$.

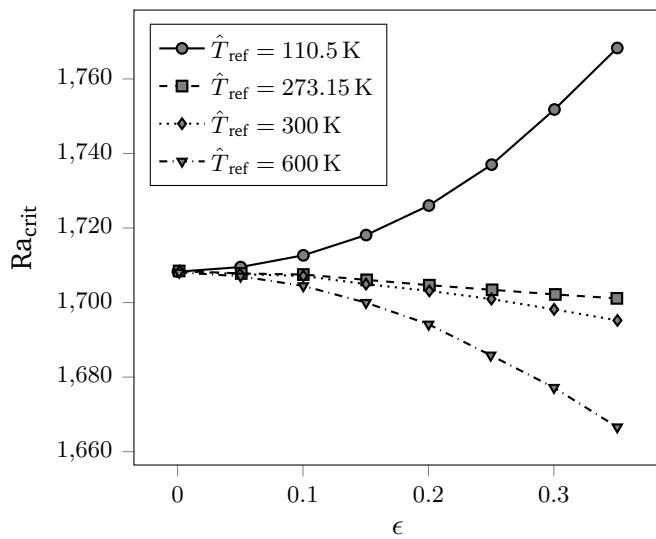


Figure 4.26: Critical Rayleigh number at different temperatures and different reference temperatures.

to conclude that, at least for small temperature differences, the low-Mach approximation has a behavior similar to that of the equations with the Boussinesq approximation.

In relation to this, it is interesting to analyze the influence of the temperature difference within the system with respect to the critical Rayleigh value. This is demonstrated in Figure 4.26, where the calculation is done for different values of the reference temperature. Clearly, for low ϵ the critical value is very close to the theoretical value obtained under the Boussinesq approximation. As ϵ increases, a larger deviation becomes apparent. This can be attributed to the dependence of the viscosity, thermal conductivity, and density coefficients on the temperature.

Finally, in Figure 4.27 and Figure 4.28 the temperature fields and streamlines obtained with the XNSEC-solver for $\epsilon = 0.5$ and $\hat{T}_{\text{ref}} = 600 \text{ K}$ for different Rayleigh numbers are shown. An interesting point to mention is the difference between the results obtained using the Boussinesq approximation and the low-Mach approximation. Comparing the results reported here with publications that use the Boussinesq approximation (Shishkina, 2021; Zhou et al., 2004), a clear

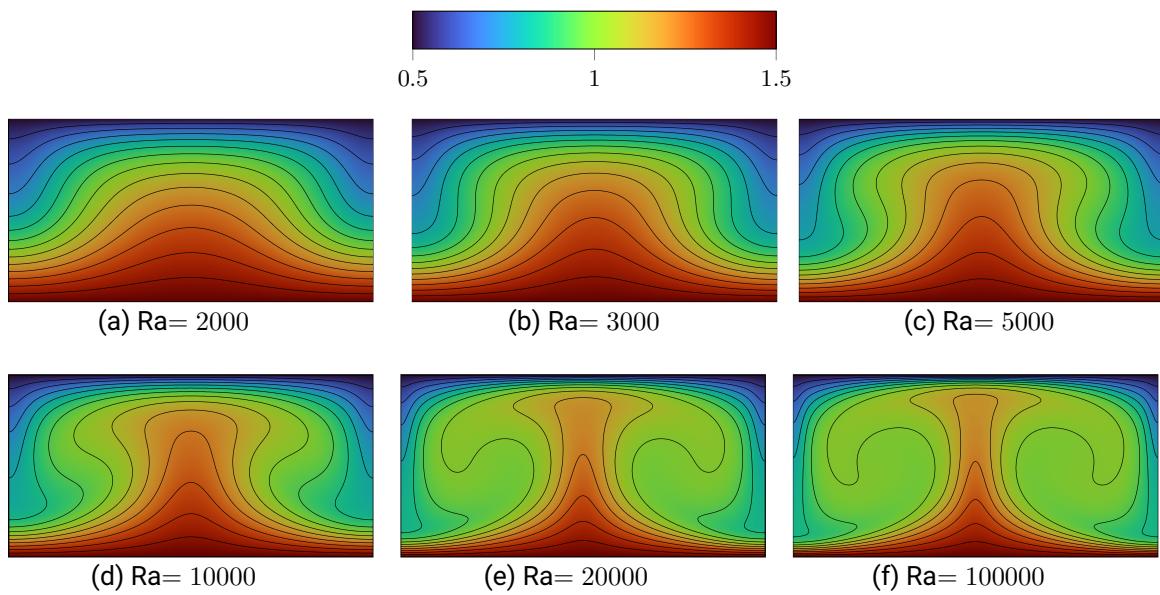


Figure 4.27: Temperature field and contours of a Rayleigh-Bénard convection roll

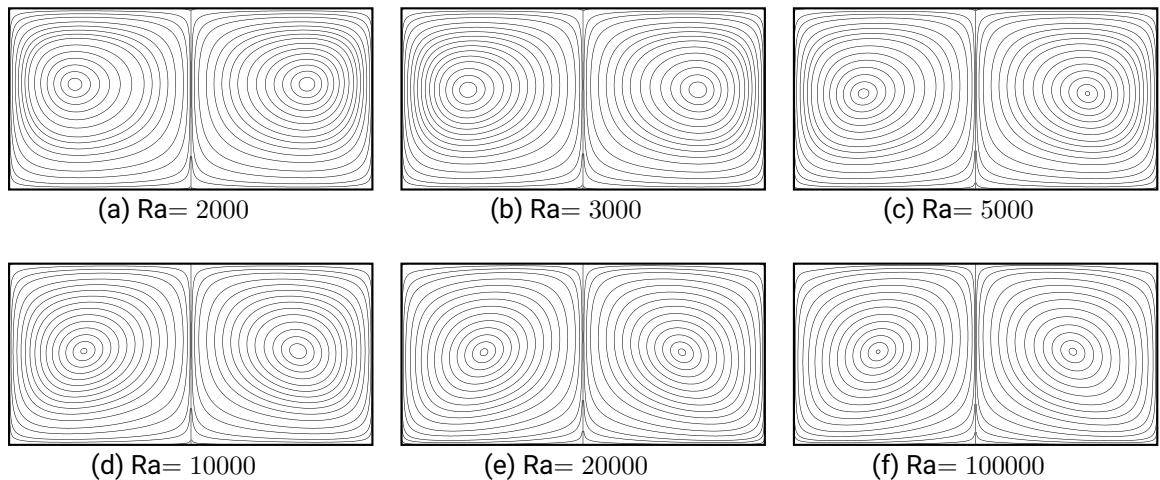


Figure 4.28: Streamlines of a Rayleigh-Bénard convection roll

difference in the streamlines is observed. In particular, the centers of the streamlines obtained with the low-Mach solver are slightly shifted towards the colder zones, while the streamlines obtained with the Boussinesq approximation do not present this deviation and remain close to the center. A possible explanation for this is that with the Boussinesq approximation the expansion effects of the fluid are ignored, whereas in the low-Mach equations this is not the case. When the latter is used, the hot fluid moves the center of the streamline towards the cold fluid.

Pressure outlet boundary condition

Now a transient calculation of the Rayleigh-Bénard configuration is done. The configuration is similar to the one described in the last part, with the difference that the boundaries of the left

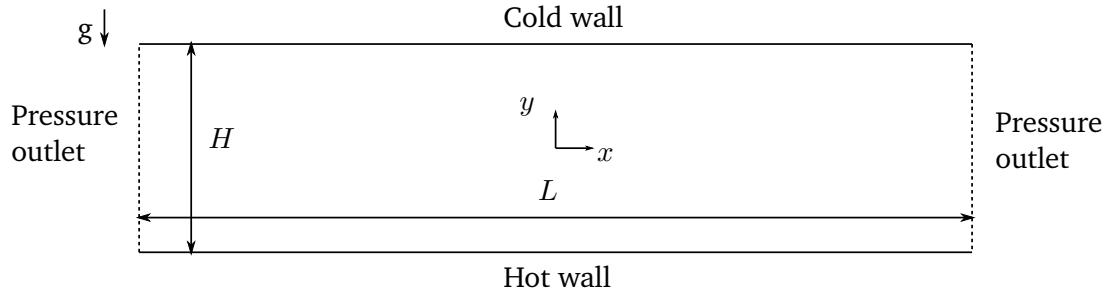


Figure 4.29: Geometry of the Rayleigh-Bénard convection with pressure outlet boundary conditions.

and right sides are now pressure outlet boundary conditions and the length L of the system is chosen considerably longer. A sketch showing the system is shown in Figure 4.29. Theoretically, an infinitely long system should be used to avoid the influence of the boundary condition to be able to adequately represent the convection rolls. The nondimensional lengths are chosen as $H = 1$ and $L = 10$. A grid with 32×320 cells is used. The polynomial degrees for the velocity components and temperature are set to four and for the hydrodynamic pressure to three. The time discretization is done again with a BDF-3 scheme and the calculation time is 150, using timesteps of $\Delta t = 0.5$. The temperatures are set to $T_h = 1.5$ and $T_c = 0.5$, with a reference temperature of $\hat{T}_{\text{ref}} = 600$ K. The Rayleigh number is $\text{Ra} = 5659$, which is above the critical value. The initial conditions are chosen as

$$u(t = 0) = 0, \quad (4.24a)$$

$$v(t = 0) = 0, \quad (4.24b)$$

$$T(t = 0) = 1, \quad (4.24c)$$

$$p(t = 0) = -\frac{\rho y}{\text{Fr}^2}. \quad (4.24d)$$

Note that no vortex is included in the initial conditions and that only a fluid at rest is considered. A perturbation-like effect caused by the pressure outlet boundaries triggers the movement of the fluid. At the first stages of the simulation the perturbations induce a vortex-like structure close to the left and right boundaries, and start gradually filling the whole domain, reaching finally a steady solution. This can be seen in Figure 4.30. Clearly in the center of the domain (far away from the outlet boundary conditions), the structure of the solution is very similar to the ones shown in the last subsection. In fact, if the domain length is chosen sufficiently large, they should be equal.

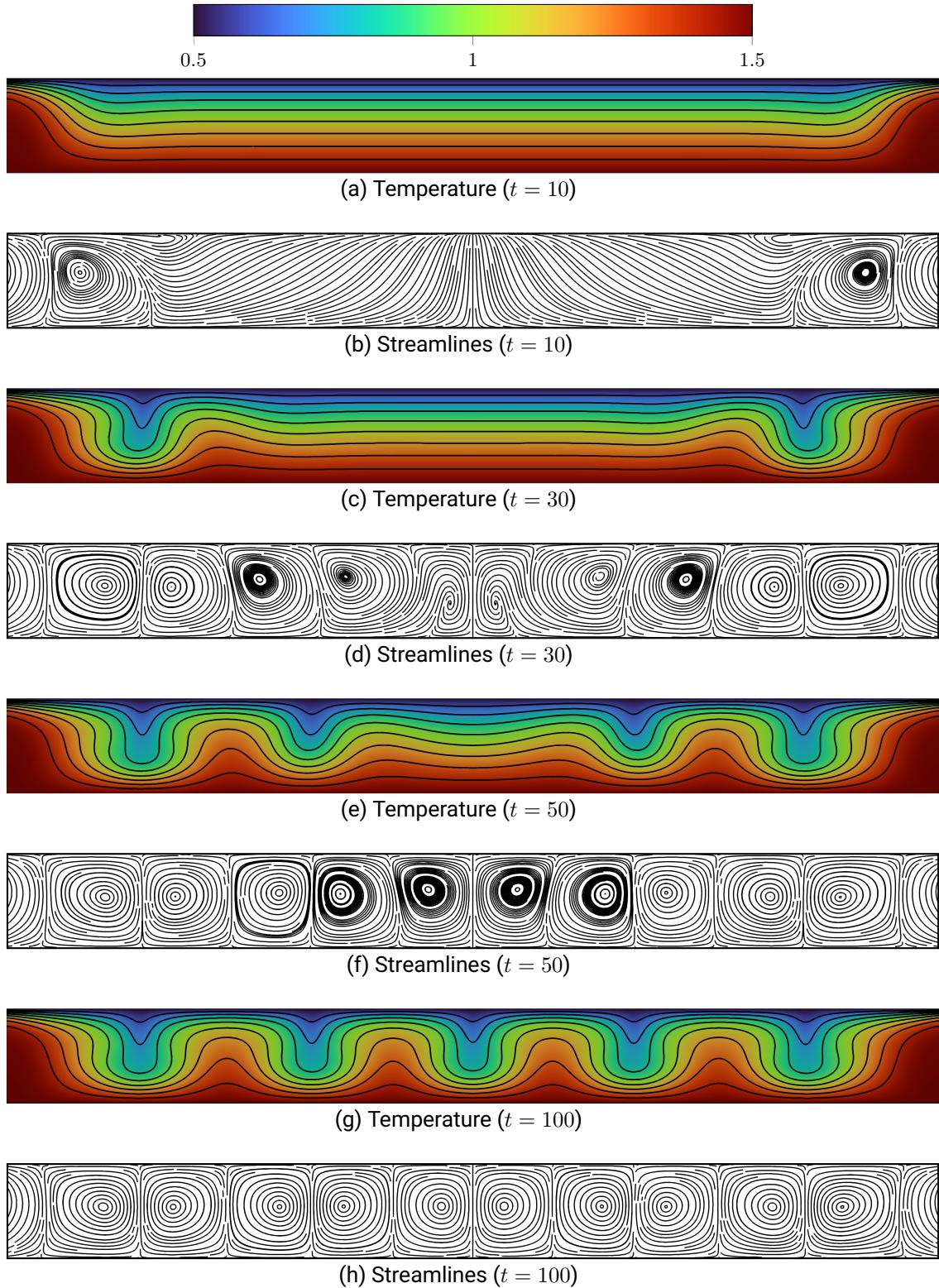


Figure 4.30: Temperature and streamlines of the Rayleigh-Bénard flow with pressure outlets.

4.3 Multi-component non-isothermal cases

Finally in this section, test cases where the whole operator presented in Chapter 3 is used, meaning that the balance equations of continuity, momentum, energy and species are considered and solved in a coupled manner, together with a equation of state and expressions for the transport parameters. For all the cases treated here, the solution of the flame sheet problem described in Section 2.2 is calculated first, and then this solution is used as an initial estimate for the solution of the finite chemistry rate problem (see Section 2.1.2). For all test cases presented in this section, a smoothing parameter $\sigma = 0.02$ was used (see Section 3.2.5).

The combustion model used for is the one-step model shown in Section 2.1. All calculations assume methane as fuel, therefore, the relevant chemical components are CH_4 , O_2 , CO_2 , H_2O and N_2 , thus $N = 5$ and $\mathbf{Y}' = (Y_{\text{CH}_4}, Y_{\text{O}_2}, Y_{\text{CO}_2}, Y_{\text{H}_2\text{O}})$. The nitrogen mass fraction Y_{N_2} is calculated according to Equation (2.23).

First in Section 4.3.1 a coflow laminar diffusion flame configuration is calculated and some remarks about the convergence behaviour of the XSEC-solver using are done. Next in Section 4.3.2 a diffusion flame in a two-dimensional counterflow configuration is simulated and compared with results from a one-dimensional configuration solved using a fourth-order finite difference solver. Finally in Section 4.3.3 the convergence rates of the fully coupled solver are investigated by studing a pseudo-one-dimensional diffusion flame configuration.

4.3.1 Co-flow laminar diffusion flame

The co-flowing flame configuration is used as a first test to assess the behavior of the solver for reactive flows applications. It consists of two concentric ducts that emit fuel and oxidant into the system, which after ignition forms a flame. This configuration has been widely studied, starting in the seminal work of Burke and Schumann, 1928 and followed by many others (see, for example, Smooke and Giovangigli, 1992; Smooke et al., 1986; Braack et al., 1997). In particular, the work from Smooke and Giovangigli, 1992 and later publications solved this configuration using a 2D-axisymmetric system and also used the flame sheet estimates to find adequate initial conditions for their Newton algorithm.

Since the solution of the axisymmetric system of equations presents numerical difficulties that are not the main concern of the present work, in this section an infinitely long slot burner configuration is considered. For that kind of configuration, cartesian coordinates describe naturally the problem.

Set-up

A schematic diagram of the configuration can be seen in Figure 4.31a. The system consists of a fuel inlet with two oxygen inlets on its sides. These inlets are separated by a finite wall thickness. The inclusion of this separation was observed to be necesary to be able to obtain a converged solution, which makes sense, since a finite separation between both inlets eases the big gradients due to strong mixing and reaction in that area. Altought the system is clearly symmetric around the axis $x = 0$, no symmetry assumption is made and the whole domain is considered for the simulation.

The lengths depicted on Figure 4.31a are set as $r_1 = 1$, $r_2 = 1.2$, and $r_3 = 11.763$. Aditinally $h = 4$ and $H = 63$. The lengths r_3 and H are set with arbitrarily large values in order to avoid

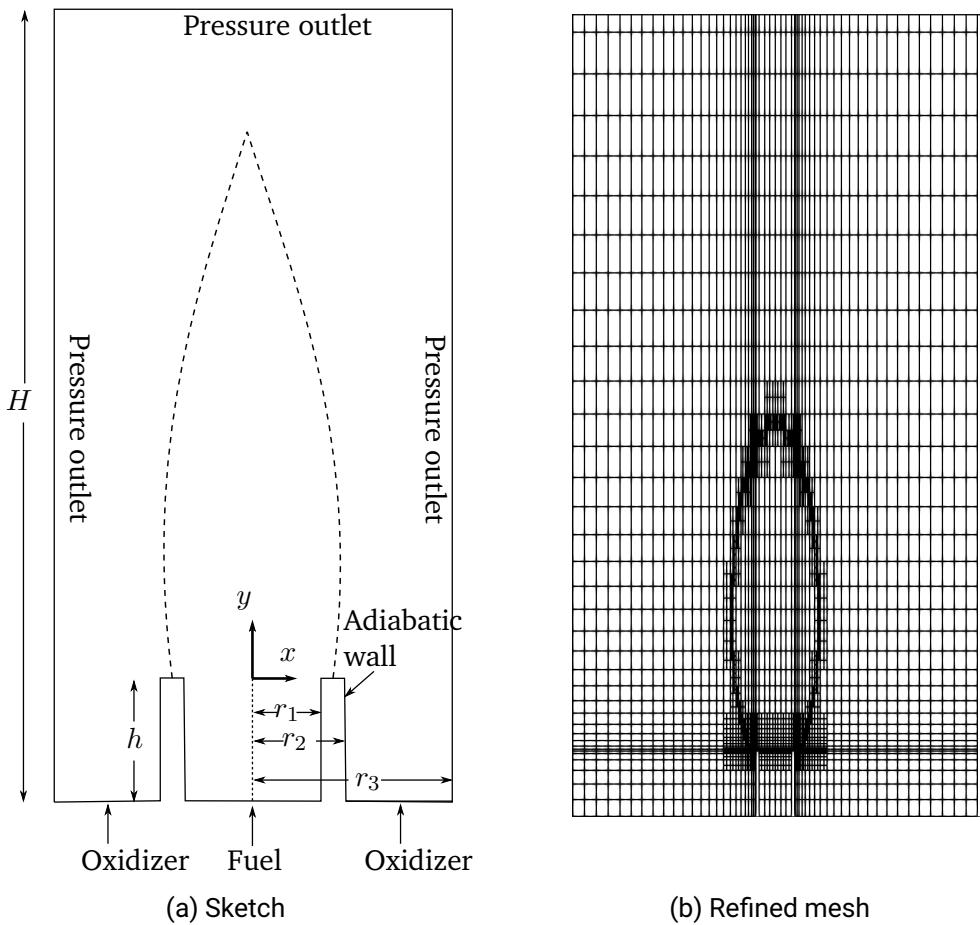


Figure 4.31: Geometry of a coflowing flame configuration (not to scale).

influence of the outer boundary conditions on the solution of the flame zone. Setting a higher value of r_3 or L did not significantly affect the results. The inlet boundary conditions are set as:

- Oxidizer inlet: $\{\forall(x, y) : y = -h \wedge x \in [-r_3, -r_2] \cup [r_2, r_3]\}$

$$u = 0, \quad v = v_O, \quad T = T^O, \quad \mathbf{Y}' = (0, Y_{\text{O}_2}^O, 0, 0)$$

- Fuel Inlet: $\{\forall(x, y) : y = -h \wedge x \in [-r_1, r_1]\}$

$$u = 0, \quad v = v^F(x), \quad T = T^F, \quad \mathbf{Y}' = (Y_{\text{CH}_4}^F, 0, 0, 0)$$

The oxidizer enters the system as a plug flow with a constant velocity of $v_O = 1$. The inlet velocity of the fuel stream v_F is a parabolic profile given by

$$v^F(x) = \left[1 - \left(\frac{x}{X_1} \right)^2 \right] v_m^F \quad (4.25)$$

with $v_m^F = 0.592$. The inlet temperatures of both streams is $T^F = T^O = 1$. Combustion of diluted methane on air is considered, with $Y_{\text{CH}_4}^F = 0.2$ and $Y_{\text{N}_2}^F = 0.8$ for the fuel stream, and $Y_{\text{O}_2}^O = 0.23$ and $Y_{\text{N}_2}^O = 0.77$ for the oxidizer stream. The superindexes F and O represent the

fuel and oxidizer inlet respectively. The pressure outlet boundary condition is the same as Equation (2.36c). Finally, the boundary conditions at the tips correspond to adiabatic walls, which are defined as in Equation (2.36b), with $\mathbf{u}_D = (0, 0)$.

The variables are nondimensionalized in the usual way. The reference length is set $\hat{L}_{\text{ref}} = 0.635 \text{ cm}$ and the reference velocity $\hat{u}_{\text{ref}} = 8.19 \text{ cm s}^{-1}$. The reference temperature is $\hat{T}_{\text{ref}} = 300 \text{ K}$. All derived variables are nondimensionalized using the air stream as a reference condition, i.e. $\hat{\rho}_{\text{ref}} = 1.17 \text{ kg m}^{-3}$, $\hat{\mu}_{\text{ref}} = 1.85 \times 10^{-5} \text{ kg m}^{-1} \text{ s}^{-1}$ and $\hat{W}_{\text{ref}} = 28.82 \text{ kg kmol}^{-1}$, giving the non-dimensional numbers $\text{Re} = 33.02$ and $\text{Da} = 2.17 \cdot 10^9$. The Prandtl number is assumed to be constant with $\text{Pr} = 0.71$. The reference heat capacity is set $\hat{c}_{p,\text{ref}} = 1.3 \text{ kJ kg}^{-1} \text{ K}^{-1}$, which is also the constant value used for the flame-sheet calculation (i.e. $c_p = 1$). The choice of this value for the heat capacity is important because it gives a solution of the flame-sheet which is similar to the actual solution of the full problem. Gravity effects are not taken into account. The transport parameters are calculated using Sutherland law with $\hat{S} = 110.5 \text{ K}$. The mixture heat capacity c_p is calculated with Equation (2.28) and using NASA polynomials for the heat capacity of each component. Finally, a non-unity but constant Lewis number formulation is used, with $\text{Le}_{\text{CH}_4} = 0.97$, $\text{Le}_{\text{O}_2} = 1.11$, $\text{Le}_{\text{H}_2\text{O}} = 0.83$ and $\text{Le}_{\text{CO}_2} = 1.39$ (Smooke and Giovangigli, 1991)

Numerical results

The purpose for simulating this case is to test the XSEC-solver in a real-application configuration, with realistic physical parameter values. In particular, it is intended to demonstrate that the strategy of using the flame-sheet solution as the initial estimate is adequate for obtaining a converged solution, even for a case where the physical properties of the system (ρ, μ, c_p) are composition and temperature dependent, and for non-unity Lewis numbers. Numerical experiments using the XSEC-solver showed that the solution of the problem is highly mesh-dependent. The presence of very high gradients in some areas requires a higher density of cells to obtain a well-resolved solution. In Figure 4.31b the actual mesh used for the solution

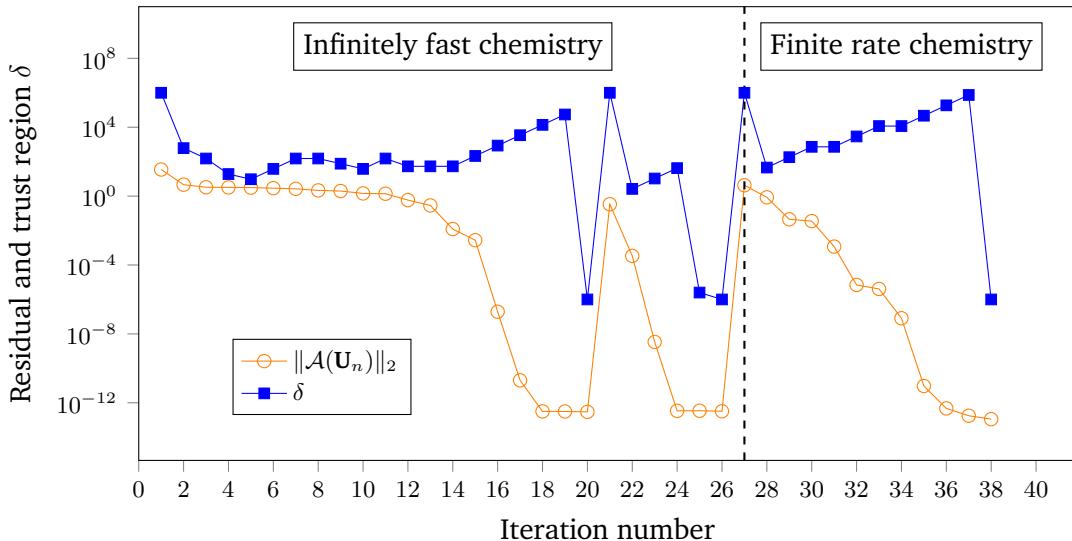


Figure 4.32: Typical convergence history of a diffusion flame in the coflowing flame configuration. A mesh refinement was done at iteration 21.

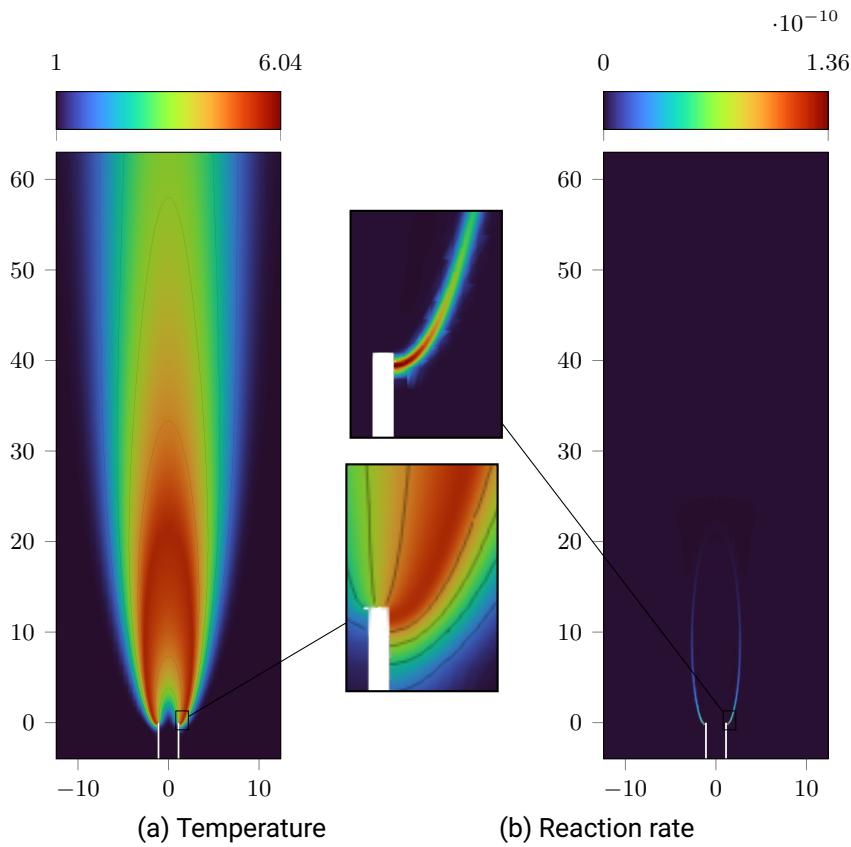


Figure 4.33: Temperature and reaction rate fields of the coflow configuration.

of the full problem is shown. A base mesh with smaller elements in the vicinity of the inlets and larger elements further away from them is used. It was observed that the complex mixing and combustion phenomena that occur in the vicinity of the inlets have a critical effect on the convergence of the solution. For this reason, a special refinement of the base mesh was done in the vicinity of the tips. Furthermore, an adequate mesh resolution at the flame location is critical. In order to avoid over-solving, an adaptive mesh refinement strategy in a pseudo-time-stepping framework was used. After obtaining a steady state solution, the mesh is refined and the calculation is started again (see Section 3.2.5). In particular, for this case, three pseudo-timesteps were performed for the flame-sheet calculation. After each pseudo-timestep, the mesh is refined in the vicinity of the flame sheet, that is, in the cells where $z = z_{st}$. Obviously, a finer grid in the vicinity of the surface $z = z_{textst}$ will be beneficial for the solution of the finite reaction rate problem if the same conditions used to derive the flame-sheet equations (namely constant c_p and unity Lewis number) are assumed. However, experiments with the XSEC-solver have shown that this refinement strategy is still beneficial for the convergence of the complete problem even with non-constant c_p and non-unity Lewis numbers.

In Figure 4.32 the convergence history using the newton algorithm presented in Section 3.2.1 is shown. The flame-sheet calculation requires 20 Newton iterations to find a solution. It is clearly seen how the residuals $\|\mathcal{A}(\mathbf{U}_n)\|_2$ decrease very slowly for about the first 14 iterations, while the parameter δ of the globalised Newton method is adapted to find an optimal value to reduce the residuals. Around iteration 14 the algorithm starts to increase δ , leading to a faster

reduction of the residuals. A solution to the problem according to the termination criteria Section 3.2.2 is found in iteration number 20. In iteration 21 mesh refinement based on the strategy mentioned above is used and now only 6 iterations are required to find a converged solution. Finally, in iteration number 27 the flame-sheet solution is used as the initial estimate for the full problem, which requires only 11 iterations to find a solution.

For the flame sheet calculation a polynomial degree $k = 2$ was chosen, resulting in a rather small system with 49,140 degrees of freedom. For the finite rate calculation $k = 4$ was used, which resulted in a system with 482310 degrees of freedom. With the above-mentioned another advantage of the approach of using the flame sheet calculation for two-dimensional simulations can be highlighted. The initial estimate can be found relatively easily for a system with few degrees of freedom. Using the solution found as the initial estimate has the consequence that Newton's algorithm for the complete problem (which has many more degrees of freedom) only needs a few iterations to find a solution.

In Figure 4.33 the obtained temperature and reaction rate fields are shown. Since for the selected inlet velocities the flame corresponds to a overventilated one, the typical jet form is observed. The maximum temperature reached corresponds to 6.04 (meaning 1812 K). Magnified plots show that the bottom part of the flame sits on the outside part of the tips. It is also appreciated the high reaction rates appearing in the area close to the inlets. This could be an explanation to why it was crucial to obtain a converged solution that the meshing in the vicinity of the inlets is finer.

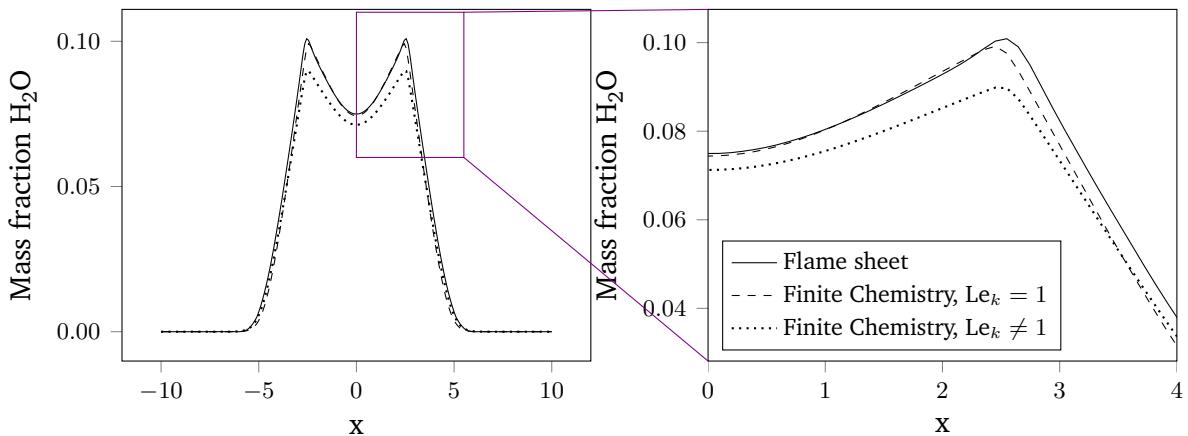


Figure 4.34: Mass fraction field of H_2O over the line $y = 10$

A question to consider is whether indeed the initialization of the finite reaction rate problem with the flame sheet provides adequate estimates for the newton algorithm. In particular for more complex problems that do not meet the assumptions made to obtain the equations of the mixture fraction problem such a systems with nonconstant heat capacity c_p or with non-unity Lewis numbers. For illustrative purposes, the simulation of the coflowing flame for unity and nonunity lewis numbers was performed. In Figure 4.34 the solution obtained for the mass fraction field of H_2O along the line $y = 10$ is shown. As expected, the solution obtained for the case with unity Lewis number is very close to the one obtained using the flame sheet. Furthermore. the case with non-unity Lewis number also presents a solution very similar to that of the flame sheet, with a small deviation in the vicinity of the zones where the chemical reaction occurs. Both finite chemistry calculations use the same initial estimate and both calculations find the converged solution after 11 Newton iterations. In all the simulations

shown in this thesis, the use of the flame-sheet estimation served as a way to initialise the finite-reaction ate problem.

The simulation of the coflowing flame shows that the strategy of using the flame-sheet as an initial condition presents an efficient way to obtain steady state solutions of combustion problems. Since the flame-sheet is only an estimate, it is possible to perform the calculations on relatively coarse grids, and use low order polynomial degrees. The obtained solution can be used as an estimate for calculations with higher polynomial degrees to find a more accurate solution of the full problem in a few iterations. A disadvantage, as already mentioned, is the choice of the c_p parameter, since an inappropriate choice of it gives a solution of the flame-sheet problem far away from the solution of the full problem. However, the user's experience and access to experimental information allows estimating this value relatively easily. It is worth mentioning that the value chosen in this section ($\hat{c}_{p,\text{ref}} = 1.3 \text{ kJ kg}^{-1} \text{ K}^{-1}$) served as an adequate estimate for all the simulations presented in this thesis.

4.3.2 Counterflow diffusion flame *

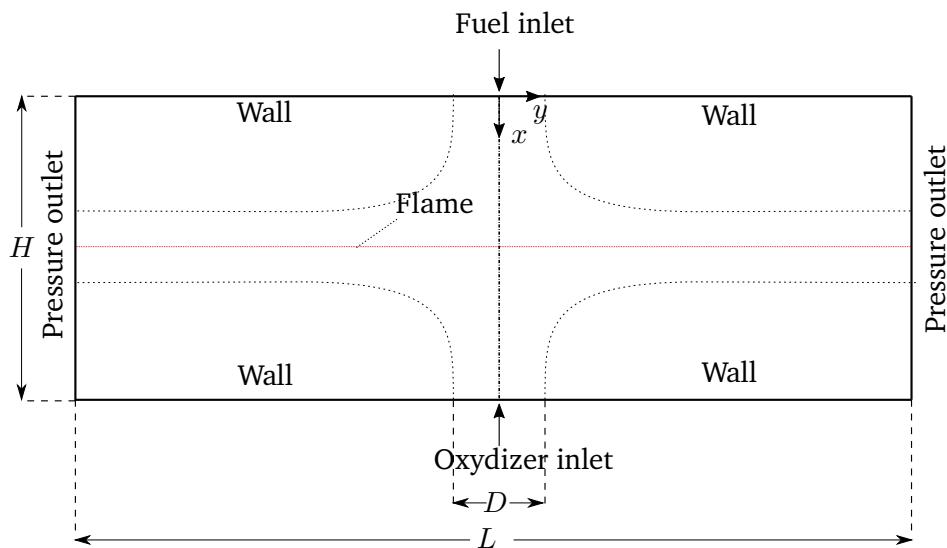


Figure 4.35: Schematic representation (not to scale) of the counterflow diffusion flame configuration.

The counterflow diffusion flame is a canonical configuration used to study the structure of nonpremixed flames. This simple configuration has been a subject of study for decades because it provides a simple way of creating a strained diffusion flame, which proves to be useful when studying the flame structure, extinction limits or production of pollutants of flames (Pandya and Weinberg, 1964; Spalding, 1961; Keyes and Smooke, 1987; Lee et al., 2000).

The counterflow diffusion flame consists of two oppositely situated jets. The fuel (possibly mixed with some inert component, such as nitrogen) is fed into the system by one of the jets, while the other jet feeds oxidizer to the system, thereby establishing a stagnation point flow. On contact and after ignition, the reactants produce a flame that is located in the vicinity of the stagnation plane. A diagram of the setup can be seen in Figure 4.35. In this section, the solution of a steady two-dimensional flame formed in an infinitely long slot burner will be

*Modified version from Gutiérrez-Jorquera and Kummer, 2022

treated. Simirlarly to the coflow configuration treated before, the infintely long slot burner configuration can be calculated naturally using cartesian coordinates.

First, as a means of verificating the solver for combustion applications, the results obtained with the XNSEC-solver for steady two-dimensional counterflow diffusion flame are compared with the solution of a simplified system of equations for a steady and quasi one-dimensional flame. Later, the influence of the inlet velocities on the maxmimum temperature is studied and finally some remarks concerning the convergence behaviour of the case counter diffusion flame are given.

The one-dimensional diffusion flame

By assuming an infinite injector diameter, a self-similar solution and by neglecting the radial gradients of the scalar variables along the axis of symmetry, it is possible to reduce the three-dimensional governing equations to a one-dimensional formulation along the stagnation streamline $y = 0$ (see the textbook from Kee et al., 2003 for the derivation). The governing equations for a steady planar stagnation flow reduce to

$$\frac{\partial \hat{\rho} \hat{v}}{\partial \hat{x}} + \hat{\rho} \hat{U} = 0 \quad (4.26a)$$

$$\hat{\rho} \hat{v} \frac{\partial \hat{U}}{\partial \hat{x}} + \hat{\rho} \hat{U}^2 = -\hat{\Lambda} + \frac{\partial}{\partial \hat{x}} \left(\hat{\mu} \frac{\partial \hat{U}}{\partial \hat{x}} \right) \quad (4.26b)$$

$$\hat{\rho} \hat{c}_p \hat{v} \frac{\partial \hat{T}}{\partial \hat{x}} = \frac{\partial}{\partial \hat{x}} \left(\hat{\lambda} \frac{\partial \hat{T}}{\partial \hat{x}} \right) + \hat{Q} \hat{\mathcal{Q}} \quad (4.26c)$$

$$\hat{\rho} \hat{v} \frac{\partial Y_k}{\partial \hat{x}} = \frac{\partial}{\partial \hat{x}} \left(\hat{\rho} \hat{D} \frac{\partial Y_k}{\partial \hat{x}} \right) + \hat{W}_k \nu_k \hat{\mathcal{Q}} \quad (k = 1, \dots, N-1) \quad (4.26d)$$

Equation (4.26). where \hat{U} is the scaled velocity and $\hat{\Lambda}$ is the radial pressure curvature, which is an eigenvalue independant of x . Again, the hat sign represent dimensional variables. The equations are written assuming a valid Fick's law and an one-step combustion model. The system of equations needs to be solved for \hat{v} , \hat{U} , \hat{T} and for Y_k , ($k = 1, \dots, N-1$). Aditonally an equation of state and expressions for the heat capacity \hat{c}_p and transport parameters $\hat{\mu}$, $\hat{\lambda}$, $(\hat{\rho} \hat{D})$ are needed. This formulation is very well known and often used for analysis of flame structure, determination of extintion points, to mention a few.

In order to assess the ability of the XNSEC-solver to simulate such a system, the solution obtained for a two dimentional configuration is compared with the solution of the quasi one-dimensional equations solved with BVP4, a fourth order finite difference boundary value problem solver provided by MATLAB (Kierzenka and Shampine, 2001). The BVP4 solver provides automatic meshing and error control based on the residuals of the solution, allowing to create with relative easyness a code that solves the one-dimensional equations.

It is important to mention some points regarding the solution of these equations using the BVP4 solver. Analogous to the problem mentioned in Section 3.2.5, the solution of the system of Equations (4.26a) to (4.26d) presents the particularity that it is possible to find multiple solutions. One of them is clearly the cold solution and another solution is the burning one. The same idea mentioned in Section 3.2.5 is also valid for the quasi one-dimensional configuration. In particular this means, that as a first step for finding a converged solution of Equations (4.26a)

to (4.26d) is to solve the system

$$\frac{\partial \hat{\rho} \hat{v}}{\partial \hat{x}} + \hat{\rho} \hat{U} = 0 \quad (4.27a)$$

$$\hat{\rho} \hat{v} \frac{\partial \hat{U}}{\partial \hat{x}} + \hat{\rho} \hat{U}^2 = -\hat{\Lambda} + \frac{\partial}{\partial \hat{x}} \left(\hat{\mu} \frac{\partial \hat{U}}{\partial \hat{x}} \right) \quad (4.27b)$$

$$\hat{\rho} \hat{v} \frac{\partial Z}{\partial \hat{x}} = \frac{\partial}{\partial \hat{x}} \left(\hat{\rho} \hat{D} \frac{\partial Z}{\partial \hat{x}} \right) \quad (4.27c)$$

together with the equation of state Equation (2.26) and expressions for the transport parameters. The dependency of the temperature and mass fractions on the mixture fraction Z is given by the Burke-Schuhmann limit. This solution can be used as a initial estimate for the solution of Equations (4.26a) to (4.26d). An inconvenience is that an initial estimate for the \hat{c}_p has to be chosen. It was observed that if the value of \hat{c}_p was chosen too big, the solver delivered solutions without a flame. For the calculations treated here $\hat{c}_p = 1.3 \text{ kJ kg}^{-1} \text{ K}$ was an adequate value that delivered the ignited solution.

It was however observed that this flamesheet solution wasnt directly useful as an initial estimation for the solution of the full system of equations. In order to help the BVP4 solver to find a coveredged solution, an intermediate step was necesary. First, the flamesheet solution was used as an initial estimate for the solution of system Equation (4.26) and the equation of state and equation for transport parameters but assuming a constant heat capacity. Once the algorithm has found a solution, it can be used for solving the same system but with a variable heat capacity according to Equation (2.28).

Set-up of the two-dimensional counterflow diffusion flame

The combustion of diluted methane with air in a two-dimensional infinitely long slot burner configuration is studied in this part. The solution is obtained by solving the system Equation (2.22), making use of the flame-sheet solution as initial estimates. The transport parameters are calculated using Sutherland law with $\hat{S} = 110.5 \text{ K}$. Gravity effects are not taken into account. The mixture heat capacity c_p is calculated with Equation (2.28) and using NASA polynomials for the heat capacity of each component.

For the comparison with the quasi one-dimensional model, three pairs of inlet velocities are considered. They are shown in Table 4.4. Here, v_m^F and v_m^O are the maximal velocity of a parabolic profile for the fuel and air inlets, respectively. Both streams enter at a temperature $\hat{T}^O = \hat{T}^F = 300 \text{ K}$. The mass composition of the fuel inlet is assumed to be $Y_{\text{CH}_4}^F = 0.2$ and $Y_{\text{N}_2}^F = 0.8$, and the oxidizer inlet is air with $Y_{\text{O}_2}^O = 0.23$ and $Y_{\text{N}_2}^O = 0.77$. Counterflow diffusion flames are usually characterized by the strain rate a . Many different definitions for it can be found in the literature (Fiala and Sattelmayer, 2014). In this work the definition of the strain

	$\hat{v}_m^F (\text{cm s}^{-1})$	$\hat{v}_m^O (\text{cm s}^{-1})$	$a(\text{s}^{-1})$	$\hat{T}^F (\text{K})$	$\hat{T}^O (\text{K})$
case(a)	4.85	12.29	34	300	300
case(b)	12.13	30.73	76	300	300
case(c)	26.69	67.62	155	300	300

Table 4.4: Maximum inlet velocity, strain and temperatures used for the counterflow diffusion flame calculations.

rate the maximum axial velocity gradient is used. The strains for the three cases mentioned above are 34 s^{-1} , 76 s^{-1} and 155 s^{-1} , respectively.

The lengths described in Figure 4.35 are $\hat{D} = 2\text{ cm}$, $\hat{H} = 2\text{ cm}$ and $\hat{L} = 12\text{ cm}$. The variables are non-dimensionalized using $\hat{L}_{\text{ref}} = 2\text{ cm}$, $\hat{T}_{\text{ref}} = 300\text{ K}$ and $\hat{p}_{\text{ref}} = 101\,325\text{ Pa}$. For each case, the reference velocity is set to $\hat{u}_{\text{ref}} = \hat{v}^O$. Again, all derived variables are nondimensionalized using the air stream as a reference condition, i.e. $\hat{\rho}_{\text{ref}} = 1.17\text{ kg m}^{-3}$, $\hat{\mu}_{\text{ref}} = 1.85 \times 10^{-5}\text{ kg m}^{-1}\text{ s}^{-1}$ and $\hat{W}_{\text{ref}} = 28.82\text{ kg kmol}^{-1}$. The reference heat capacity is set $\hat{c}_{p,\text{ref}} = 1.3\text{ kJ kg}^{-1}\text{ K}^{-1}$.

Under this conditions, the Reynolds numbers are $\text{Re} = 156$, $\text{Re} = 390$ and $\text{Re} = 858$, for the low, medium and high inlet velocities respectively. The Dahmkoler numbers are $\text{Da} = 4.6 \cdot 10^9$, $\text{Da} = 1.8 \cdot 10^9$ and $\text{Da} = 8.3 \cdot 10^8$. The Prandtl number is assumed to be constant with $\text{Pr} = 0.71$. A non-unity but constant Lewis number formulation is used, with $\text{Le}_{\text{CH}_4} = 0.97$, $\text{Le}_{\text{O}_2} = 1.11$, $\text{Le}_{\text{H}_2\text{O}} = 0.83$ and $\text{Le}_{\text{CO}_2} = 1.39$ (Smooke and Giovangigli, 1991). The system is considered open, then the thermodynamic pressure is constant and set to $p_0 = 1$.

The boundary condition of the inlets are,

- Oxidizer inlet: $\{\forall(x, y) : y = 0 \wedge x \in [-D/2, D/2]\}$

$$u = 0, \quad v = v^O(y), \quad T = 1.0, \quad \mathbf{Y}' = (0, Y_{\text{O}_2}^O, 0, 0)$$

- Fuel Inlet: $\{\forall(x, y) : y = H \wedge x \in [-D/2, D/2]\}$

$$u = 0, \quad v = v^F(y), \quad T = 1.0, \quad \mathbf{Y}' = (Y_{\text{CH}_4}^F, 0, 0, 0)$$

The pressure outlet boundary condition is the same as Equation (2.36c). The pressure outlet boundaries are placed far away of the center of the domain, in order to decrease the effect on the centerline. Placing the boundary further away did not change appreciably the results. Finally the boundary conditions at the walls are defined as in Equation (2.36b), with $\mathbf{u}_D = (0, 0)$ and a constant temperature $T = 1.0$.

In Figure 4.36 the solution profiles for the case (a) are shown. The used mesh was obtained by a process of mesh refinement. The base mesh is initially created with a larger concentration of elements in the center of the domain. The points of intersection from the velocity inlet and wall boundary conditions are also refined, which was observed to improve the robustness of the algorithm. Similarly to the coflowing flame (Section 4.3.1), during the solution algorithm of the flame sheet problem, mesh is additionally refined around the flame sheet making use of a pseudo-timestepping setting. As expected, a stagnation flow develops and a flame forms close to it. For this strain rate, a maximum temperature of $T = 6.05$ is obtained (1815 K). This big increase in the temperature is also reflected in a big decrease in the density field, where a decrease of almost six times on the density values is appreciated. This change of density also provokes the acceleration of fluid, as observed in Figure 4.36b.

In Figure 4.36k the reaction rate given by Equation (2.24) is plotted. It is interesting to see that the actual reacting zone is very small, which clearly demonstrates why adequate meshing is necessary to capture the steep gradients resulting from the strong and highly localized heat sources. Finally, and as expected, the fuel and oxidizers field seem to only be found on either side of the flame. Althought it can not be seen here, some reactant leaking occurs, meaning that there exists a small zone where both especies coexist. This point will be adressed later.

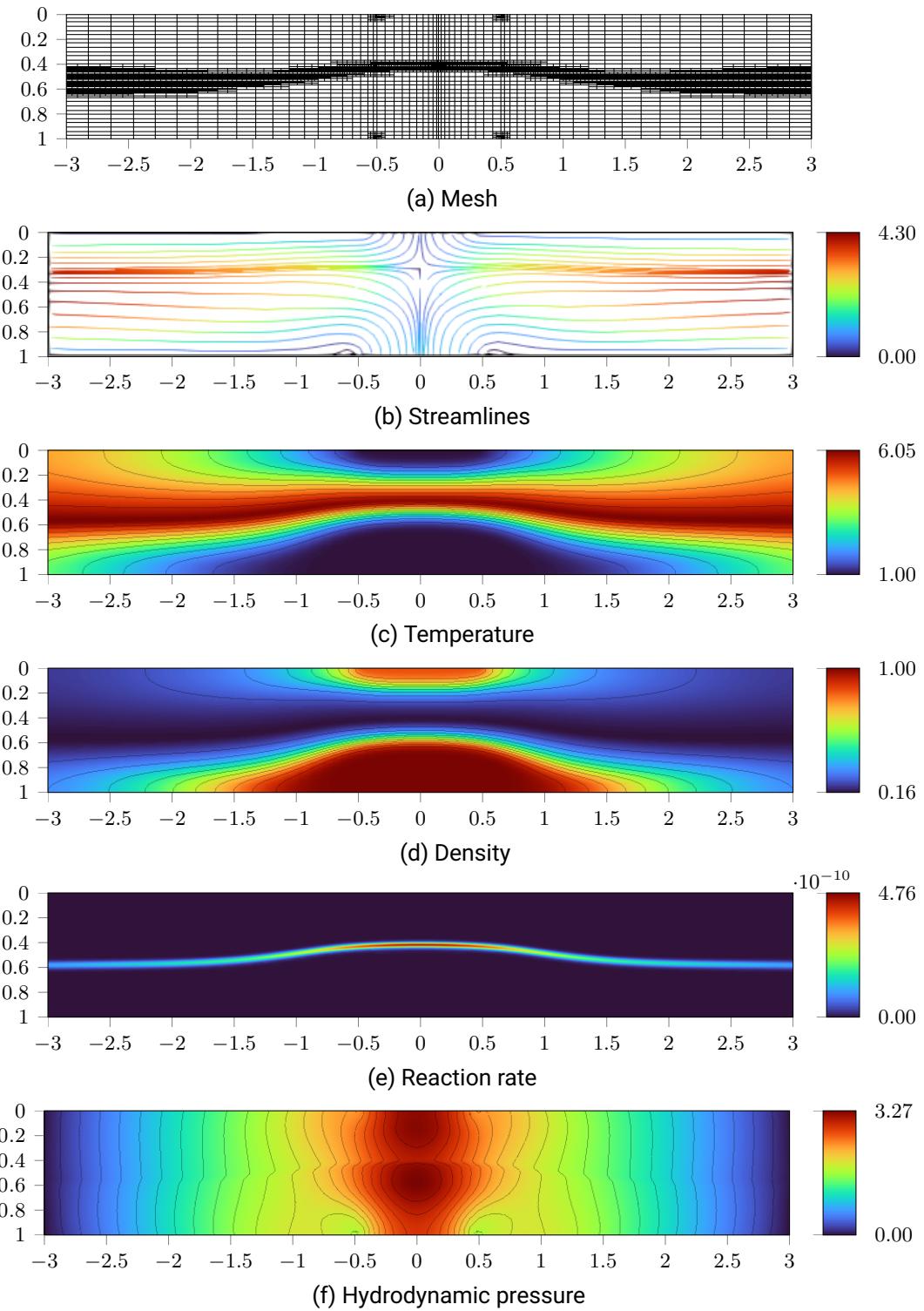


Figure 4.36: Nondimensional solution and derived fields of the counterflow flame configuration for case (a).

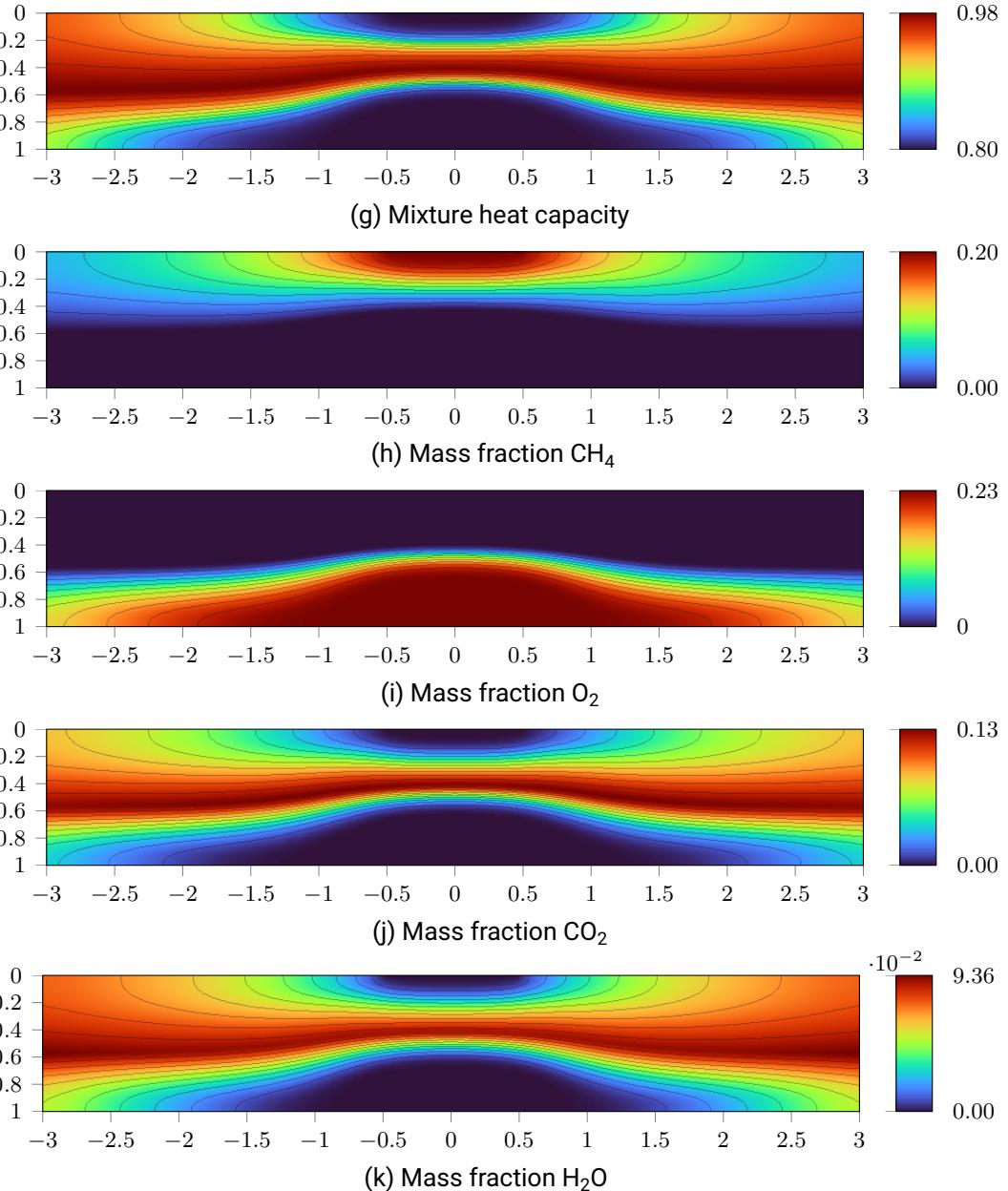


Figure 4.36: Nondimensional solution and derived fields of the counterflow flame configuration for case (a) (continued).

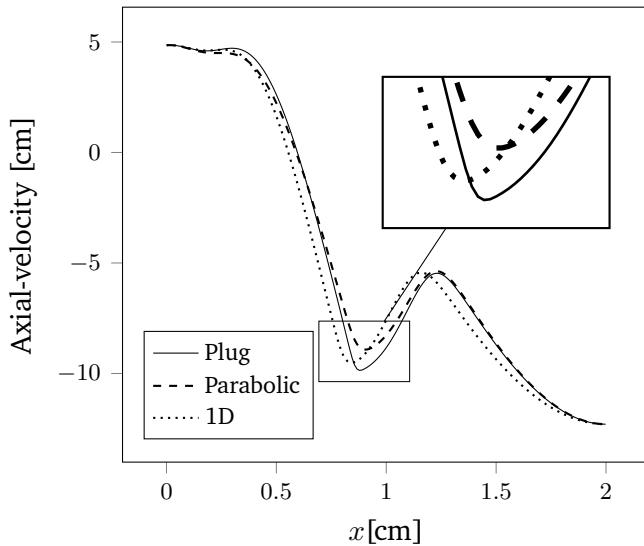


Figure 4.37: Velocity profiles of the counterflow diffusion flame for parabolic and plug inlet boundary conditions.

Comparison of two-dimensional and the quasi one-dimensional counterflow flames

In this section a comparison of the results obtained with the XSEC-solver for a two dimensional counterflow diffusion flame, and the results obtained with the BVP4 solver for a quasi one-dimensional flame is done. The comparison of both set of results is done along the centerline of the domain (see Figure 4.35). In this section, only dimensional variables will be considered. The transport parameters, chemical model and the equation of state are exactly the same for both formulations. For all calculations in this section, a polynomial degree of four is used for the velocity components, temperature and mass fractions. A polynomial degree of three is used for the pressure. This resulted on systems with approximately 439000 degrees of freedom.

The choice of the type of velocity boundary conditions for the inlets requires some attention. Different possibilities exist to describe the velocity profiles. One possibility is to characterize the velocity boundary conditions by assuming a Hiemenz potential flow, where a single parameter defines the flow field. Other possibilities are also a constant velocity value (plug flow) or a parabolic profile, allowing to define different velocity values for each jet inlet. The effect of boundary conditions on the flame structure has been studied by Chelliah et al., 1991 and Johnson et al., 2015, where it was concluded that both plug and potential are able to adequately describe experimental data.

The question whether a plug or parabolic flow profile allows a better representation of the quasi one-dimensional equations was treated in the work from Frouzakis et al., 1998. There is stated that the one and two dimensional formulations deliver very similar results, provided that the inlets of the two-dimensional configurations are uniform. Furthermore, preliminary calculations with the XSEC-solver showed that the selection of a plug flow or parabolic have an influence on the solution, as shown in Figure 4.37. Based on these results, the plug flow boundary condition is adopted for all following test cases.

In Figure 4.38 a comparison of the axial velocities calculated with the XSEC-solver and the one-dimensional solution is shown. While for the high strain case the results agree closely, for lower strains a discrepancy is observed. Recall that the derivation of the one-dimensional

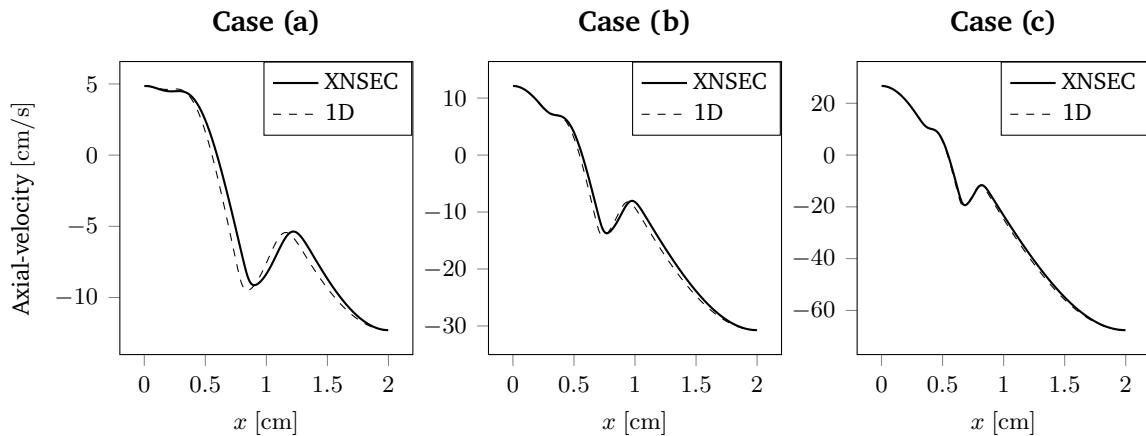


Figure 4.38: Comparison of the axial velocity calculated with the XNSEC-solver and the one-dimensional approximation.

approximation assumes a constant velocity field incoming to the flame zone in order to obtain a self-similar solution. In the case of the two-dimensional configuration presented here, the border effects do have an influence on the centerline, which disrupts the self-similarity. This effect is more pronounced for low velocities, which explains the discrepancy between curves.

Similarly, In Figure 4.39 the temperature and mass fraction fields are presented. Again, a discrepancy is observed for low strains, but results show a good agreement for higher inlet velocities. It can also be observed how, as expected, at higher strains a significant leakage of oxygen across the flame is present. This is a typical behaviour of a flame that is getting closer to its extinction point Fernandez-tarrazo et al., 2006.

This is a drawback from usual one-step models with constant activation temperature, because they tend to overpredict fuel leakage. This behaviour is not appreciated in the one-step model with variable activation temperature used here. In Figure 4.40 the comparison is shown for the configuration (c) between the mass fractions fields obtained using a chemical model with variable kinetic parameters given by Equations (2.19) and (2.20) and other with constant kinetic parameters using $\hat{T}_a = \hat{T}_{a0}$ and $\hat{Q} = \hat{Q}_0$. The oxygen leakage obtained by using the chemical model with variable parameters is evident, confirming

In Figure 4.41 the maximum temperature obtained in the centerline for different strain rates is plotted. Qualitatively speaking, the solution obtained with the XNSEC-solver agrees with the expectations. As the strain rate increases, the maximum temperature decreases (see Figure 3.3). On the other hand, the comparison of values obtained with the XNSEC-solver and those of the quasi one-dimensional approximation clearly shows a discrepancy in the results. For low strain rates this discrepancy is small, being for $a = 20 \text{ s}^{-1}$ only 10K, approximately a difference of 0.5%. As the strain rate increases so does the discrepancy. For $a = 200 \text{ s}^{-1}$ the difference is almost 50K, which is a 9% disagreement. A similar behaviour is also reported in Frouzakis et al., 1998, where a difference of 50K was reported.

It is worth noting that the XNSEC-solver wasn't able to find a converged solution for $a > 202 \text{ s}^{-1}$, and the newton algorithm stagnates. This is most probably a sign of underresolution of the mesh, and that the used refinement strategy did not help for such high strain rates. A better mesh refinement strategy is necessary for calculating the flame at conditions near the extinction point. Moreover, for high strain rates the flame will be far from the thermochemical equilibrium, and it is likely that the solution obtained for the flame sheet will be far away from

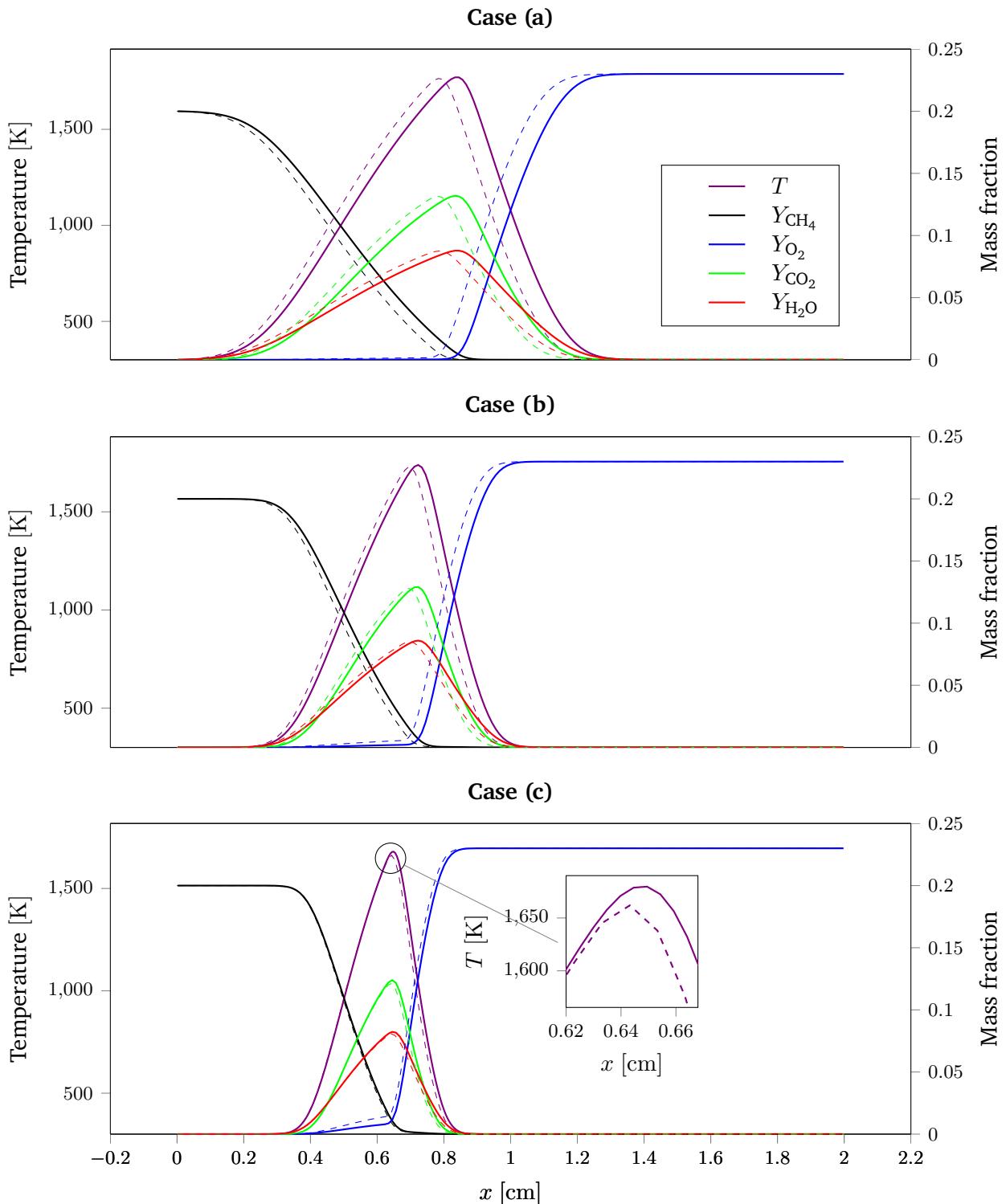


Figure 4.39: Comparison of temperature and mass fraction fields obtained with the XNSEC-solver (solid lines) and the one-dimensional approximation (dashed lines).

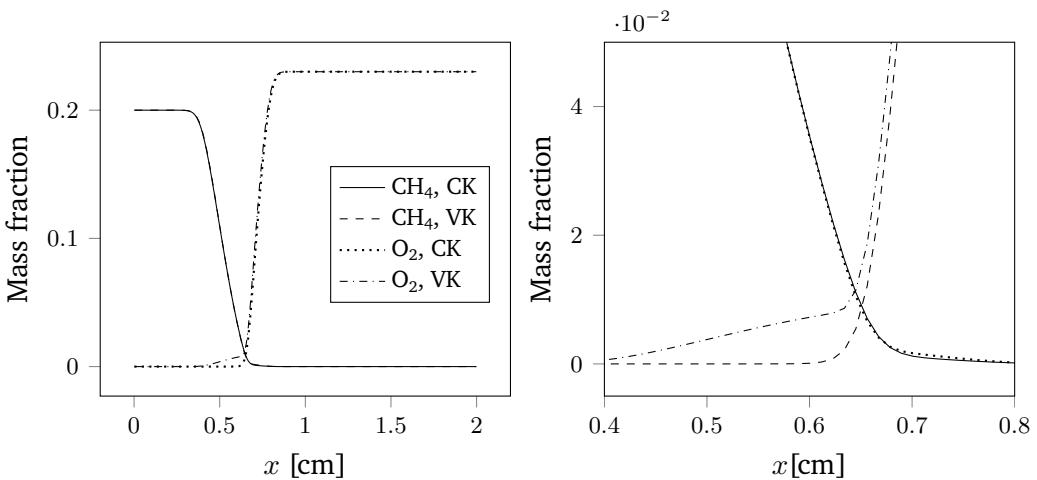


Figure 4.40: Mass fraction profiles of methane and oxygen along the centerline of a counterflow diffusion flame configuration using variable kinetic parameters (VK) and constant kinetic parameters (CK). Right picture is zoomed in near the flame zone.

the solution with finite rates. A possibility would be to use one of the well-known continuation methods (see for example Nishioka et al., 1996) to progressively move in the direction of the extinction point. Obviously, the Homotopy Methodology presented in Section 3.2.4 can be visualized as one of those methods, and would be useful when looking for solutions of systems that are close to the extinction point. A complexity that arises then is how to create a dynamical mesh that is suitable for obtaining the intermediate solutions while searching for the final result in a robust way. This issue is beyond the scope of this thesis, and may be the subject of future research.

The difference between the results obtained for the two-dimensional configuration and the quasi-one dimensional approximation could be explained by some condition within the 1D system assumptions being violated in the 2D configuration. It is known that in addition to the boundary conditions, the ratio between the slot width and the separation between the two slots (D/H) also has an influence on the solution, and that a high ratio is desirable (Frouzakis et al., 1998). Another point that was not addressed here is whether the boundary conditions chosen for cold walls have an effect on the solution along the centerline. Other possibilities could have been using outlet boundary conditions or an adiabatic wall. It is nevertheless expected that its effect on the centerline would not be big. The points mentioned here should be addressed in future work.

Temperature convergence study

Similar to problems presented in earlier sections, the presence of singularities caused by non-consistent boundary conditions causes a degenerative effect on the global error values, making a global convergence study for this configuration is problematic. However, it is still possible to study the behaviour of some characteristic point value under different conditions to prove the mesh independence of the solution.

In Figure 4.42 it is shown how the maximum temperature along the centerline obtained for configuration (b) behaves under different mesh resolutions and polynomial degrees. Values for $k = 1$ are not shown, because for this range of cell elements the maximum temperature

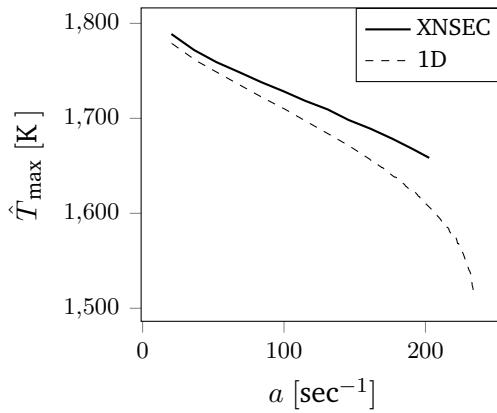


Figure 4.41: Maximum centerline temperature of a counterflow flame for different strains.

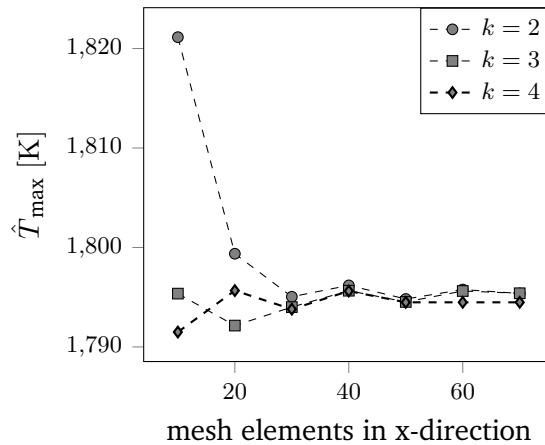


Figure 4.42: Convergence study of the maximum value of the temperature for the counterflow diffusion flame configuration.

value was of the order of 60K higher than the ones depicted here. The temperature tends to a limit value, and it's possible to observe how this value is reached already for coarse meshes when using a polynomial degree of three or four. For $k = 2$ the temperature also tends to a limit value, but at a slower rate when compared to $k = 3$ or $k = 4$.

In the next section a simplified one-dimensional flame configuration will be used in order to be able to realize a h -convergence study of the whole system operator.

4.3.3 Chambered diffusion flame

The chambered diffusion flame configuration has served as a model for many theoretical studies related to diffusion flames (Matalon and Metzner, 2010; Rameau and Schmidt-Lainé, 1985; Matalon et al., 1980). A sketch of the configuration can be seen in Figure 4.43. Fuel is injected at a constant rate into the bottom of a small insulated chamber, while oxidant diffuses into the system against the direction of flow. Constant conditions at the outlet of the chamber are achieved by a rapid renewal of the flow of oxidant. Under these conditions a planar flame forms far away from the walls, which allows a one-dimensional description of the flame structure. The fuel inlet into the chamber is modelled with a velocity inlet boundary

condition Equation (2.36a), while the flow outlet at the top is considered an outlet as given by Equation (2.36d). Since we are interested in the flame in wall distance, it is sufficient to set the remaining boundary conditions as periodic boundaries. This effectively transforms the problem into a pseudo two-dimensional configuration.

In this test case we study the combustion of a $\text{CH}_4\text{-N}_2$ mixture with air. The thermodynamic pressure \hat{p}_0 is set equal to an ambient pressure of 101 325 Pa. The inlet velocity of the fuel jet is set to 0.025 m s^{-1} and its mass composition is $Y_{\text{CH}_4}^0 = 0.2$ and $Y_{\text{N}_2}^0 = 0.8$ while air has a composition $Y_{\text{O}_2}^0 = 0.23$ and $Y_{\text{N}_2}^0 = 0.77$. The temperature of the fuel and air feed streams is 300 K. The length of the system L is equal to 0.015 m. For this configuration an h -convergence study is conducted, where uniform Cartesian meshes with 5×2^6 , 5×2^7 , 5×2^8 , 5×2^9 and 5×2^{10} cells are used. The polynomial degrees are varied from 1 to 4 for velocity, temperature and mass fractions, and from 0 to 3 for pressure. Errors are calculated using the finest mesh as a reference solution. The results are shown in Figure 4.44 for variables u_x , T , Y_{CH_4} and p . The convergence results for other variables are similar and not shown here. We observe the expected slope increase with increasing polynomial degrees. For low polynomial degrees the orders of convergence are very close to the theoretical values. However for higher polynomial degrees we observe a slight deterioration of the convergence rate.

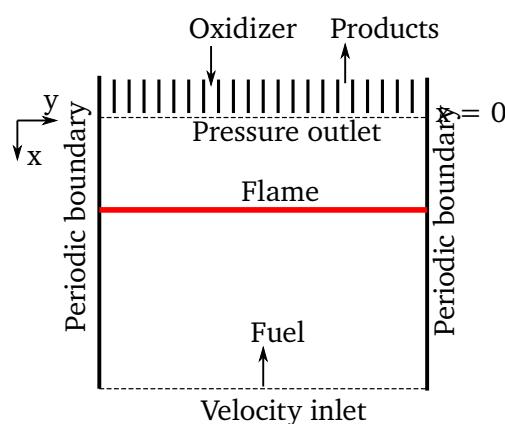


Figure 4.43: Schematic representation of the chambered diffusion flame configuration.

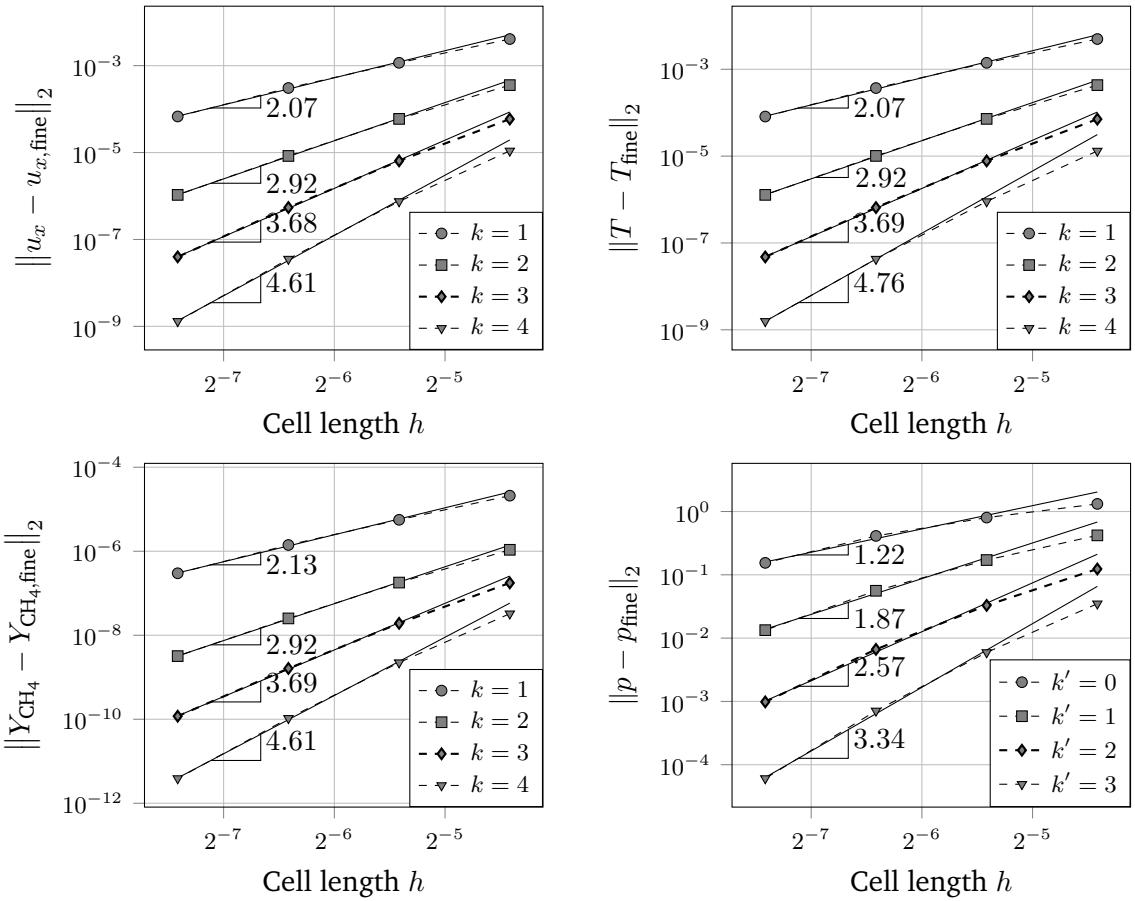


Figure 4.44: Convergence study for the chambered diffusion flame configuration.

5 Conclusion

In the present work we have shown the discretization using the DG method for the reactive low-Mach equations. A mixed order formulation has been used, where velocity, temperature and mass fractions are represented by polynomials of degree k , and pressure by polynomials of degree $k - 1$. The system obtained from the discretization was solved by means of a Newton-Dogleg type method. Additionally, a homotopy strategy for solving highly nonlinear systems was introduced and used for some of the presented test cases. For the reactive test cases the concept of the flame sheet estimate was demonstrated to be a useful and computationally cheap way of initializing the finite reaction rate combustion calculations. The solver was used to calculate three different benchmark configurations, one without combustion and two cases with combustion. The first of these is the differentially heated cavity. This benchmark case was solved for varying Rayleigh numbers, spanning from $\text{Ra} = 10^2$ to $\text{Ra} = 10^7$. It was observed that for cases with Rayleigh number larger than 10^5 the use of our homotopy strategy was necessary to ensure convergence. Velocity and temperature profiles as well as thermodynamic pressure and Nusselt number were compared with a reference solution, obtaining very satisfactory results, thus validating our implementation of the method for variable density systems. An h -convergence study was presented for the differentially heated cavity, obtaining the expected convergence rates up to $k = 4$, where some degeneration on the rates was observed. Furthermore the counterflow diffusion flame configuration was analyzed, with which we intended to test the implemented chemistry model in conjunction with our solver. The results obtained with BoSSS were compared with results obtained by solving the self-similar one-dimensional representation of the counter diffusion flame configuration for varying strain rates. While for low strains some discrepancies between results were observed, the difference narrowed for high strains, which can be explained by the influence of the border effects on the centerline results for a two-dimensional configuration. Finally, the chambered diffusion flame configuration was used to study the convergence rates of our method. It was shown that, as expected, the convergence rates increase when using higher degree polynomials, but with some deterioration compared to the theoretical expected convergence. In future work the implemented solver is intended to be used in conjunction with our extended-DG solver Kummer, 2017; Kummer et al., 2021; Krause and Kummer, 2017 in order to study multiphase reactive systems such as droplets.

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