Direct numerical simulations in engine-like geometries

A thesis submitted to attain the degree of

DOCTOR OF SCIENCE of ETH ZURICH

(Dr. sc. ETH ZURICH)

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2014
Abstract

Increasing fuel costs and alternative power sources like hydrogen for fuel-cells and electricity for battery-electric vehicles increase the pressure on Internal Combustion Engine (ICE) development towards cleaner and more efficient combustion processes. Improvements of existing combustion systems by "downsizing" or new combustion concepts like Homogeneous Charge Compression Ignition (HCCI) have the potential to further reduce the in-cylinder emissions in combination with increased efficiencies, but problems in controlling the combustion process and in increased stresses on the engine structure still persist. In order to implement the new engine concepts, improved understanding of phenomena such as cycle to cycle variations and the wall heat transfer are necessary.

Due to its high spatial and temporal resolution, Direct Numerical Simulations (DNS) can provide unique insights into the physical processes in ICEs, which are to the best of our knowledge completely lacking in literature.

The objective of this thesis is to perform large-scale DNS simulations in a laboratory-scale engine-like geometry, which has been studied experimentally by Morse et al. [1]. After the implementation of the Arbitrary Langrangian-Eulerian (ALE) formulation and the introduction of a temporally variable mean pressure term into the energy equation in the framework of the spectral element code Nek5000, multiple cycles in the valve/piston
assembly were calculated and excellent agreement with experimental mean and rms velocities was found [1]. The evolution of the flow field showed significant cycle to cycle variations (CCVs) and the cause-and-effect relationships were investigated in detail. Main driving forces of the CCVs were found to be the interaction between the radial velocity at Top Dead Center (TDC), the jet trajectory during intake and the stability and orientation of the central vortex ring at Bottom Dead Center (BDC). Statistical post-processing of the flow field provided the full Reynolds stress tensor, integral length scales and the turbulent kinetic energy, which can be used for validation of existing RANS or LES turbulence models used in ICE simulations and to guide the development of novel models.

In the second step, the effect of compression on flow, temperature and composition fields was investigated by closing the valve at BDC. The analysis focused on the investigation of the hydrodynamic and thermal boundary layers and the unsteady wall heat transfer during compression. The global wall heat transfer was found to be strongly influenced by the decreasing kinematic viscosity, leading to increased velocity and temperature gradients at the walls. The local wall heat flux distribution was found to correlate strongly with the wall normal velocity, transporting hot gases towards and cold gases away from the walls. In density weighted wall-normal units, collapsing profiles of the velocity and thermal boundary layers were observed and in agreement with the literature [2] no logarithmic boundary layer profile was found, which is the base for many wall heat transfer models used in ICEs.

For the setup and conditions considered in this work, the initial conditions for temperature were quickly forgotten and the spatio-temporal evolution of the temperature field and heat transfer during compression was almost fully determined by the flow field at BDC and the wall temperature.
Zusammenfassung


Für die in dieser Arbeit untersuchten Bedingungen zeigte sich, dass die Temperaturverteilung am unteren Totpunkt nur einen geringen Einfluss auf die thermische Stratifikation während der Kompression hat. Entscheidend für die Temperaturverteilung sind das Strömungsfeld und die Wandtemperatur.
First and foremost, I would like to thank my advisor Professor Konstantinos Boulouchos for his continuous support throughout the whole work. He guided me with his great experience and his door was always open when I needed help. The trust he put in me helped me to grow both as a researcher and a person. I also would like to thank Dr. Christos Frouzakis for his support especially at his continuous insistence on working accurately and documenting the results in a structured way. Many thanks to Professor Andreas Dreizler for his willingness to act as my co-supervisor and for very interesting discussions about experiments and DNS in engines during my visit in Darmstadt.

Very special and warm acknowledgment goes to Dr. Yuri Martin Wright for many fruitful discussions and personal advices. I learned a lot from him in scientific and less scientific senses (e.g. he showed me how much fun ski tours can make). I would like to thank Professor Ananias Tomboulides for insightful discussions during his visits to ETH. Without his help for the implementation of the ALE formulation and the variable dp/dt term the work in this form would not be possible.

Special thanks go to my ex-office-mate Dr. Andrea Brambilla for introducing me into the DNS code and to my other colleagues for creating a very friendly and stimulating environment. Furthermore I would like to thank several former master and semester students (Jann Koch, Rennan
Hu, Fabian Müller and Cyrill Mandanis), who helped extending my work towards a more practical direction.

This work was performed with the financial support of the Swiss National Science Foundation (SNF), Project No. 200021 135514 and computing resources were provided by the Swiss Center for Scientific Computing (CSCS) under project number s189. Special thanks to Dr. Jean Favre for his support in visualization the results.

Finally, very special thanks go to my wife Christina and my family, who supported me tremendously during the good and bad times of the thesis. They are the center of my life.
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Chapter 1

Introduction

1.1 Motivation

A large fraction of today’s worldwide energy demand (82% according to [7]) is covered by combustion. Although the power production based on alternative sources like e.g. solar energy becomes more important, combustion systems will remain the most important energy source in the next decades [8]. Especially in the transportation segment, the fraction of energy production based on combustion will remain high, due to the high energy density of fossil fuels. Main applications are gas turbines used in aircrafts and Internal Combustion Engines (ICEs) which are commonly used in large ships and land vehicles. However, combustion of fossil fuels is associated with two major problems for the environment. First, during combustion different types of pollutants are produced (NO$_x$, soot, or unburnt hydrocarbons), which have deleterious effects on the environment. Secondly, the concentration of the main combustion product CO$_2$ correlates with the worldwide increasing average temperatures [9].
1. **Introduction**

Although emissions per engine have been significantly reduced during the last two decades, an additional reduction of emissions will be imposed by regulation laws. In contrast to other emissions, \( \text{CO}_2 \) is a regular combustion product and can only be reduced by using fuels with a low C/H ratio (\( \text{CH}_4 \) or \( \text{H}_2 \)) or by increasing the engine efficiency. In addition, increasing fuel costs and alternative electrical- and fuel cell approaches for passenger cars increase the pressure in the ICE development towards cleaner and more efficient combustion processes.

In order to fulfill these requirements, the existing engine types should be improved. One possible way is the "downsizing" concept, where the displaced volume of an ICE is reduced but the power output is kept constant due to higher intake pressures. The reduced engine weight and frictional losses result in an overall increased efficiency. Limitations of this approach are increased stresses on the engine structure and knocking at low engine speeds.

New combustion concepts like the Homogeneous Charge Compression Ignition (HCCI) have the potential to further reduce the in-cylinder emissions in combination with increased efficiency [10]. The relatively higher efficiency can be achieved by increased compression ratios, absence of throttling losses and thermodynamically-favorable nearly-isochoric combustion. The reduced \( \text{NO}_2 \) and soot emissions result from the relatively low peak combustion temperature attained by typically lean mixtures or high External Gas Recirculation (EGR) rates and well-mixed operation. Problems for the practical use of compression-ignition concepts arise from difficulties
in controlling the ignition timing and in increased CO and unburnt hydrocarbon emissions, which are attributed to temperature and/or mixture inhomogeneities close to the cylinder walls [11].

In order to further improve the efficiency, reduce emissions and make new engine concepts applicable, an improved understanding of the underlying physics in internal combustion engines is necessary. Physical effects which have a strong influence on emissions and efficiency of different ICE types are up to now only partially understood. These effects include Cycle to Cycle Variations (CCVs), flow and temperature behavior close to engine walls and naturally occurring thermal stratification during the compression stroke [10, 12, 13]. The main reason for this lack of knowledge is that the origin of these phenomena is strongly connected to the complex turbulent flow in internal combustion engines, which is up to now very challenging to access using experimental or simulation methods.

On the simulation side, even the currently emerging Large Eddy Simulation (LES) models for engine flows exhibit large uncertainties with respect to the sub-grid scale models particularly in the proximity of walls, which have a strong influence on the global flow field. Therefore the validity of LES simulations in ICEs depends on validation based on experimental data. Over the last decades valuable insights into the turbulent flow field of ICEs were achieved using experiments based on optical methods, like Particle Image Velocimetry (PIV) or Laser-Induced Fluorescence (LIF). However, limitations in terms of insufficient spatial resolution and scanning of the whole domain still persist. In particular, the flow and temperature fields
close to walls, the high frequency part of the turbulent kinetic energy, or the
dissipation can be measured only to a limited extent and with significant
experimental effort, and is associated with high costs.

A possible alternative can be Direct Numerical Simulations (DNS),
which solves the flow field directly without any modeling assumptions. The
results can be considered as a high-fidelity numerical experiment [14] pro-
viding unique insight into the physical processes in ICEs. The data can
provide an excellent validation platform for existing ICE models. Up to
now, the model constants are tuned based on simple setups (e.g. homoge-
neous turbulence simulations in periodic cubic domains [15]), which differ
substantially from real engine geometries. Furthermore, the physical under-
standing gained can assist in the development of novel modeling tools on an
engineering-level for single processes like e.g. the engine wall heat transfer.

The principal limitation of DNS is its high computational cost, which
scales exponentially with the engine speed. Due to this according to Merker
[16] approaching the flow field in ICEs with DNS is not possible in the near
future. But in this work it is shown that using highly scalable numerical
tools on currently available computational resources DNS simulations in
engine-like geometries are possible.

1.2 Aim of the work

The aim of this work is to perform large scale DNS in engine-like geome-
tries under engine-like conditions. The first step is the development and
validation of a method for simulating complex, moving geometries with variable mean pressures based on the spectral element code Nek5000 [17] extended by a plugin for low Mach number combustion [18]. This includes the construction of complex grids using the meshing software Cubit [19], their conversion to Nek5000 format, the implementation of an Arbitrary Langrangian-Eulerian (ALE) approach for the so-called $P_n - P_n$ formulation based on the work of Ho [20], and the introduction of a temporally-varying mean pressure term into the energy equation.

The developed code is employed to simulate multiple cycles in the valve/piston assembly experimentally investigated by Morse et al. [1]. The setup has been selected for different reasons: Firstly, experimental data are available for the intake and exhaust stroke for validation. Secondly, the axisymmetric geometry allows averaging in azimuthal direction, which reduces the computational costs significantly. Finally, many of the important features of the flow dynamics (intake jet - breakup, interaction of the jet flow and shear layers with the walls) in the investigated setup are expected to be similar to real engine flows. Following the validation of the newly developed code against experimental data, the physics in the flow field are analyzed with emphasis on the cause-and-effect relationships of CCVs in the simulated setup. In addition, the highly resolved data are statistically analyzed to extract quantities for the development and validation of advanced turbulence models for engine simulations.

The next aim is to study flow, temperature and composition fields during the compression stroke. The analysis is motivated by the question
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how the unsteady hydrodynamic and thermal boundary layers evolve during compression and how they affect thermal stratification. Of special interest is the investigation of the unsteady engine wall heat transfer. Aim is to gain an improved understanding about the physical processes, which is needed for the development of novel engine wall heat transfer models.

1.3 Thesis Structure

The thesis is organized as follows. First, the state of the art in engine diagnostics and modeling is summarized in chapter 2. Chapter 3 discusses the mathematical model and the numerical methodology employed in the solver. The focus lies on the description of the code extensions which are the implementation of the ALE formulation in the $P_n - P_n$ approach and the introduction of the variable pressure term. Chapter 4 turns to the multiple cycle analysis of the flow field in the valve/piston assembly. The chapter reports the comparison with experimental data, the detailed description of the flow field, the statistical analysis of the turbulent flow field and the investigation of the cause-and-effect relationships of CCVs. The evolution of the flow, temperature and combustion during the compression stroke is discussed in chapter 5. Emphasis is placed on the velocity and thermal boundary layer and the unsteady wall heat transfer. Finally, chapter 6 briefly summarizes the main conclusions and highlights the implications of this work.
Chapter 2

Literature review

The flow field has a large impact on efficiency and emissions of ICEs, through its effect on wall heat losses, species mixing, thermal stratification, cycle to cycle variations and thus on the overall combustion process. In this work, the flow, temperature and composition fields related to the conventional four stroke engine concept, shown schematically in figure 2.1, are investigated.

Figure 2.1: Schematic of the four strokes in a internal combustion engine [3].
2. Literature review

The main driving force affecting the flow field in the confined geometry is the moving piston. During the intake stroke the fluid enters the cylinder through the valve(s), forming hollow jet flows. By interaction with the walls, the jet forms large organized flow structures like tumbling or swirling motions, which can be seen as vortical structures or vortex rings. During intake, the turbulent jet break up leads to increased turbulence levels, but turbulence dissipates quickly with the reduced piston speed towards BDC. The flow field evolution during intake can be considered as a sequence of interacting basic flow types like the aforementioned hollow jet flow and vortex ring. Although single flow types are well documented in the literature, little can be found on their interaction. During compression the upward-moving piston increases the density, resulting in a decreasing kinematic viscosity and reduced turbulent length scales. The flow field is mainly defined by the vortical structures from the intake stroke and the imposed velocity due to the upward-moving piston. Close to TDC, large scale fluid motions may have insufficient volume to maintain their form and they create small scale vortices, increasing the turbulence level shortly before combustion. In case the piston is designed to produce a squish flow, the turbulence level is additionally increased by an organized fluid motion towards the cylinder center. During expansion the downwards moving piston results in an attenuation of turbulence and any surviving fluid motions. Finally, during the exhaust stroke products of the combustion are pushed out of the cylinder, leaving residual fluid motions at TDC, which influence the flow during the next cycle.
2.1 State of the art in engine diagnostics and modeling

In this chapter, an overview about experimental and simulation methods for assessing flow, temperature and composition fields in ICEs is presented in section 2.1. Section 2.2 reviews cycle to cycle variations from the applied and fundamental point of view. Finally, in section 2.3 the literature about boundary layers and wall heat transfer in ICEs is presented.

2.1 State of the art in engine diagnostics and modeling

Measurements of the ICE flow, temperature and species fields are very challenging. Main problems on the experimental side arise from the difficulty to access the whole domain, short observation times and rapidly changing thermodynamic properties. In addition, ICE test rigs are very complex systems, and challenging to control accurately.

Experimentally, turbulent flows can be investigated point-wise with Laser Doppler Velocimetry (LDV) or with 2- and 3-D PIV techniques. Important early applications at Imperial College employed optically accessible motored model engine configurations. In one of the first LDV applications to engine flows, Morse et al. [21] investigated the influence of two head (straight pipe and angled annular port) and two piston (flat and cylindrical bowl in piston) geometries on the mean and fluctuating flow field in a motored valve-piston assembly. It was found that although the inlet arrangement and the incoming jet trajectory had a strong effect on the flow patterns, the bowl did not have a noticeable effect. The influence of swirling
motion on the flow characteristics were investigated by placing the open port off-center and increasing the port angle [22]. Two swirl levels were imposed by vanes upstream of the valve section and mean and rms velocities in the axial and radial directions were measured revealing increasing anisotropy with increasing swirl level. More complicated geometries were also investigated and the LDV research activities during that period are reviewed in Arcoumanis and Whitelaw [23]. In the works of Lorenz and Bopp [24, 25] cycle-resolved measurements in a spark-ignited, four-stroke, flat-piston engine with one off-center intake port operating at speeds up to 2000 \( \text{rpm} \) provided data on cyclic variability and turbulence. Dimopoulos [26, 27] performed simultaneous three-component LDV measurements in a motored pancake two-valve engine operating at speeds between 600 and 1500 \( \text{rpm} \) to obtain, in addition to mean and rms velocities, normal and shear Reynolds stresses at different swirl levels.

During the last decade, LDV was gradually replaced by PIV measurements which provide instantaneous two- or three-dimensional velocity fields at sufficient resolution to compute vorticity and strain rate [28]. The application of PIV in engines was possible due to substantial progress towards higher temporal resolution. Reuss et al. [29] applied planar PIV to a motored, four-stroke engine to obtain instantaneous velocities and the components of the strain rate with a spatial resolution of approximately 1 \( \text{mm} \). The low repetition rates for flow field measurements at that time allowed for only one exposure per cycle. Recently, new laser and camera developments increase the pulse and frame rates up to several kHz [30–32]. Using
a PIV system with a temporal resolution of 1°CA at 1000 rpm, Müller et al. [32] investigated the temporal development of large scale flow structures and their variation from cycle to cycle. In addition, the turbulent kinetic energy was calculated based on the flow field on planar slices. The recent work of Baum et al. [33] employed tomographic PIV to measure the flow field in a 3D subdomain within the cylinder. The turbulent kinetic energy $k$ calculated from the three velocity components revealed distinct differences compared to $k$ values obtained from 2D velocity information, especially in the region of the inlet jet during intake. An overview of high-speed PIV for the measurement of in-cylinder flows and sprays can be found in Towers and Towers [34].

Insight into temperature and composition fields in ICEs can be obtained using high-speed Laser-Induced Fluorescence (LIF) measurements, a spectroscopic method measuring the fluorescence of different tracer gases. A review of tracer-LIF diagnostics in practical combustion systems can be found in [35], where the fundamental concepts of how to apply quantitative measurement techniques to study fuel concentrations, temperatures and fuel/air ratios in ICEs are discussed. The behavior of different tracers like e.g. ketone, toluene and bi-acetyl with respect to pressure and temperature changes is described in detail and the potential of alternative approaches like absorption, Raman scattering and Rayleigh scattering is presented. Recent LIF works to measure temperature and composition in ICEs are reported in [36–40]. In these studies the field distributions were obtained on vertical or horizontal slices with spatial resolutions of approximately 0.4 mm.
In contrast to Peterson et al. [39], the measurements of Snyder et al. [37] and Kaiser et al. [40] showed increasing thermal stratification towards TDC, which in Dec et al. [36] and Dronniou et al. [38] is attributed to turbulent transport of cold gases from the cylinder wall to the bulk gas. Snyder et al. [37] found the species mixing process to be very efficient, resulting in a relatively fast homogenization of the fuel/air mixture during compression, despite the increased thermal stratification. Very recently, Peterson [41] measured simultaneously flow and temperature fields in a gasoline direct injection engine by combining toluene-LIF thermometry and PIV. The focus lied on the investigation of how the droplet evaporation during injection affects the temperature field. It was found that the bulk-flow motion-driven mixing reduces the temperature gradients but does not completely homogenize the temperature fields at TDC.

Despite recent progress in optical diagnostics, inherent limitations in the efficient scanning of entire flow fields with sufficient spatial resolution - down to the smallest scales and particularly in the proximity of walls - still persist. Features of the high frequency part of the turbulence kinetic energy spectrum and the associated interactions with larger scales can be uncovered only with heavy experimental effort.

On the modeling side, Reynolds Averaged Navier Stokes (RANS) simulations typically employing variants of the two-equation $k-\varepsilon$ model [42,43] are routinely performed nowadays for engine flows. The results have provided very useful contributions towards understanding of ICE flows, but also showed difficulties in predicting the physics for variable operating con-
2.1. State of the art in engine diagnostics and modeling

ditions or geometries [44]. In addition, since RANS calculations compute time or ensemble averages phenomena specific to individual engine cycles such as misfire or knock, which can limit performance and efficiency, cannot be captured.

To overcome these shortcomings, Large Eddy Simulations (LES) are increasingly used to study turbulence phenomena in internal combustion engines. One of the first LES simulations in ICEs was performed by Haworth [45], who used an in-house code to perform LES simulations of the axisymmetric piston/cylinder assembly considered here at a turning speed of 200 \( \text{rpm} \). Good agreement was obtained with the LDV measurements for two of the three experimentally investigated piston positions, but it was found that LES could not properly simulate transitional effects like the jet breakup process. More recently, Liu and Haworth [46] used the same setup to test different subgrid scale models (Smagorinsky and one-equation \( k-l \) models) and mesh resolutions. The influences of model constants and integration time steps were also investigated and a statistical analysis was presented. Similar agreement with the experimental data was obtained as in [45], and it was found that no combination of the tested model-mesh parameters could improve the agreement for all compared quantities. The strong sensitivity of mean and root-mean-square (rms) quantities to variations in subgrid models pointed to the importance of further developments in this area.

Moureau et al. [47] implemented an ALE approach in the AVBP code [48] and simulated the flow field in a square piston experiment [49]. Thboois
et al. [50] compared LES simulations with experimental LDV measurements in a sudden expansion setup. The results showed good agreement for mean and rms velocities, but in the swirling cases differences from the LDV measurements were observed. Enaux et al. [51, 52] simulated the flow field in real ICE setups and compared the predictions with experimental PIV measurements. Good agreement for the mean velocities was obtained, while small differences were observed in their variance. The progress and open questions concerning the application of LES to engine flows were recently reviewed by Rutland [53]. It was pointed out that it is worth using more complex subgrid scale models as they can lower the grid resolution requirements significantly. In general it is stated that LES is capable of adequately describing the unsteady flow field in internal combustion engines. However, even the most advanced LES models are subject to uncertainties with respect to subgrid scale models, particularly in the proximity of walls which are prominent in confined geometries.

In contrast to LES and RANS, Direct Numerical Simulations (DNS) solves the Navier-Stokes equations directly without any modeling assumptions. Thus, it provides an accurate description of the turbulent flow field, and may be considered as high-quality numerical experiments [14]. However, due to the high computational cost associated with resolving all pertinent scales, few simulations in complex geometries with moving boundaries can be found in the literature. Güntsch [54, 55] studied the effect of compression on artificial isotropic turbulent flow fields in a 3-D cylinder. A wide range of statistical quantities (mean and fluctuation quantities, probability sepa-
rations, two-point correlations, turbulent length scales, statistical moments of third or fourth order and energy density spectra) were investigated to describe the effect of compression on the turbulent flow field. The production and dissipation terms in the turbulent kinetic energy and the components of the Reynolds stress tensor were discussed in detail. It was found that the majority of the turbulent kinetic energy created during compression is related to the axial compression rate, while shear stresses have only a minor effect. However, a comparison with LDV measurements showed poor agreement for fluctuating quantities, which was attributed to uncertainties in the measurement positions and in the initial conditions.

Under reactive conditions, the ignition characteristic of processes like HCCI has been investigated by using artificial stratified turbulence and temperature fields without simulating complex and moving geometries. Several recent studies employed 2D DNS to describe the influence of weakly thermally stratified initial conditions on the HCCI autoignition chemistry (e.g. [56–61]). In Hawkes et al. [56] and Chen et al. [57] the auto-ignition behavior was investigated for different artificial turbulent and temperature initial conditions of a lean ($\lambda = 0.1$) homogeneous H$_2$/air mixture at 41 atm. The fluctuations of zero-mean velocity and constant mean temperature fields were initialized using a Passot-Pouquet spectrum [62], which requires the most energetic wavenumber and the fluctuation velocities as input parameters. Temperature fluctuations were found to have a strong effect on combustion mode, timing and duration of the heat release. Increased thermal stratification leads to advanced ignition, longer combus-
2. Literature review

tion processes and a significantly higher fraction of fuel consumption due to deflagration instead of homogeneous ignition. However, under real engine conditions turbulent quantities like the integral length scales or fluctuation velocities are difficult to measure or estimate and are expected to vary significantly within the domain. It is thus difficult to estimate how the artificial stratified turbulence and temperature fields reflect the conditions in ICEs. In addition, with the use of artificial initial fields the prominent influence of the walls on flow and temperature is not taken into account.

2.2 Cycle to cycle variations

Flows in ICEs depend on engine type and operation conditions and are characterized by a high level of Cycle to Cycle Variations (CCVs). For several reasons, CCVs are very problematic for the design and operation of ICEs. High levels of cyclic variability result in large cyclic differences in the combustion process, which in extreme cases can lead to knocking or misfire and reduce the engine efficiency by up to 10\% [63]. In addition, CCVs also have an influence on pollutant formation, since exhaust composition and temperature change from cycle to cycle.

Possible sources of CCVs are variations in the fluid motion, the supplied amount of fuel, the air and exhaust gas recirculation (EGR), spatial mixture inhomogeneities at the spark plug, and the discharge characteristics of the spark plug [3]. The relative importance of these factors is hard to estimate since they influence each other and depend on the operating conditions. Experimentally, several studies have identified the previously named
2.2. Cycle to cycle variations

different sources and influencing factors of cyclic fluctuations [64–66]. A review of the experimental work concerning CCVs in engines is given in Ozdor et al. [63]. Despite significant recent progress especially in the field of laser diagnostics in internal combustion engines (see, for example Fajardo and Sick [31], Müller et al. [32]), the investigation of CCVs faces several difficulties: first, it is difficult to control the boundary and operating conditions in a real engine setup and second, up to now optical access is limited to planes or thin cuboids within the cylinder.

During the last 15 years, the use of Large Eddy Simulations of ICEs provided new insights into CCVs. Reviews on LES in ICEs setups can be found in Rutland [53] and Celik et al. [44]. In one of the first LES application in engine-like geometries by Haworth [45], significant CCVs in the flow field were observed, despite the use of identical boundary conditions for each cycle. The variations were attributed to large length-scale long-time-scale turbulent structures, the cause-and-effect relationships of which were not discussed in detail. Vermorel et al. [13] and Enaux et al. [52] used LES to perform multiple-cycle calculations in an engine setup, which was carefully designed in order to obtain well-defined boundary conditions. A correlation between the central tumble position and the burning duration was observed, which was attributed to cyclic differences in the local flow field around the spark plug at ignition timing. However, in the aforementioned works no information about the origins of the large scale flow variations is reported.

The flow in internal combustion engines can be considered as a sequence of different basic flow types: starting at Top Dead Center (TDC),
the downward moving piston draws fluid into the cylinder and creates a hollow jet as the gas flows through the valve. During the intake stroke, the jet trajectory is strongly influenced by the valve position, the angle and thickness of the valve channel and the engine walls, which cause the formation of large vortical structures (e.g. tumble or swirl flows). Since to the best of our knowledge no fully resolved flow data in engine-like geometries are available, in the following the existing literature for jet flows and vortex rings related to ICE flows is summarized.

The hollow jet flow is related to the well-documented turbulent planar jet flow, since in ICEs the diameter of the intake valve is usually significantly larger than the gap between the valve and its seat even at full valve lift. In a planar jet, the turbulent flow field changes significantly depending on the distance to the nozzle exit. Kelvin-Helmholtz instabilities in both sides of the shear layers are formed in the first phase after the jet leaves the nozzle. At a certain axial distance from the nozzle the instabilities cause the breakup of the jet, resulting in the formation of smaller turbulent structures. In the experimental studies of Heskestad [67] and Gutmark and Wygnanski [68], hot-wire anemometry was used to measure the evolution of mean and fluctuation velocities in the self-similar region of the jet. It was found that the evolution of the spreading rate and centerline velocity are very sensitive to the conditions in the nozzle as well as the external flow field. This finding is very relevant for the flow field in ICEs, since the initial conditions of the hollow jet flow during intake are the leftover fluid motions from the previous cycle.
2.2. Cycle to cycle variations

One of the first DNS of flow and mixing behavior of a turbulent planar jet was performed by Stanley et al. [69]. The mean and rms velocities were compared to experimental data and coherency, vorticity and auto-spectra were reported. The highly-resolved DNS data showed that the mixing process in the jet shear layers is dominated by large-scale engulfing of surrounding fluid. In contrast to this, small scale mixing has a stronger effect close to the jet core and in the self-similar region. The recent review by Mahesh [70] presents an overview of the interaction of jets with cross flows. This is also relevant for engine flows, where the jet interacts with the remaining in-cylinder flow field from the previous cycle. The review summarizes the literature on mean jet trajectories, vortical structures created by the jet flow, mixing and stability behavior for incompressible and compressible jets, which are discussed in the context of several practical applications like industrial flow mixers.

The physics of large scale flow structures occurring in ICEs (e.g. tumble or swirl motions) can be related to the description of vortex rings. A direct comparison of vortex rings occurring in ICEs with those typically investigated in the literature is difficult, since the vortex formation process differs significantly and vortex rings in ICEs are strongly influenced by the time-varying geometry. An overview on vortex rings can be found in the review paper of Shariff and Leonard [71], which analyses the vortex ring formation process, the dynamic behavior of laminar and turbulent vortex rings and the interaction between vortex rings and walls. Vortex rings under laboratory conditions are most commonly formed by piston-cylinder setups,
which push a certain amount of fluid through a nozzle [71]. In the study of Glezer et al. [72], a piston forced the fluid through a cylindrically shaped valve, to create a doughnut-shaped vortex ring. The vortex formation process was studied for different Reynolds numbers, cylinder-valve diameter ratios, nozzle exit angles and nozzle exit speeds. A transition map was reported which, based on the chosen geometry and boundary condition, can predict whether a laminar, a transitional or a turbulent ring regime will be created. A recent study investigated the behavior of vortex rings in cross flows [73], which is closely related to ICEs where also the jet during intake interacts with the remaining cross flow from the previous cycle. The main result is again a map reporting different vortex ring structures depending on the velocity ratio of the jet vs. the cross-flow. For cross flow/jet velocity ratios below two no coherent vortex ring structures were observed, since the cross flow inhibits the roll-up of the nozzle boundary layer at the leading edge. For velocity ratios above two, depending on the stroke ratio two vortex ring structures could be identified. Lower stroke ratios resulted in asymmetric vortex rings, while higher stroke ratios yielded an asymmetric vortex ring accompanied by a trailing column of vorticity. Vortex ring breakdown and reconnection events can be found in the review papers of Lucca-Negro and O’doherty [74] and Kida and Takaoka [75].

For a deeper understanding of CCVs in ICE fundamental knowledge about this two flow types is necessary in order to understand how they interact with each other.
2.3 Boundary layer and wall heat transfer

Wall heat transfer in ICEs is a very complex process. Within 10 ms the flux can vary from close to zero to up to 10 MW/m² and local peaks of up to 5 MW/m² within 1 cm can be observed [12]. During the engine cycle strong variations of thermodynamical and chemical properties have a significant influence on the boundary layer structure. In addition, the valve and piston movement induces a very complex, unsteady, turbulent and cyclic varying flow field, which strongly influences the wall heat transfer.

The engine heat transfer is important for the efficiency and pollutant emissions in ICEs, since the boundary layer contains a substantial amount of the in-cylinder mass (10 - 20 %). This has especially for Otto and HCCI engine concepts a substantial impact on efficiency and unburnt hydrocarbon emissions. In addition, the local heat transfer is strongly influencing thermal stresses on the engine structure, which can have a large impact on engine design. Hence, an improved understanding of the engine heat transfer, which can lead to the development of more predictive models, is very important for future engine design.

2.3.1 Experiments and DNS

During the last decades many experimental investigations have been conducted studying wall heat transfer and velocity boundary layer in ICEs. The most common approach to experimentally derive wall heat fluxes is the measurement of instantaneous wall temperatures using thermocouples. The heat flux at discrete points at the engine walls is calculated based on
the one-dimensional heat conduction equation using the measured instantaneous wall temperature and the temperature of the cooling water as boundary conditions. An overview of thermocouple measurements can be found in the wall heat transfer review paper from Borman and Nishiwaki [12]. According to the review, thermocouple measurements are excellent validation data for heat transfer models, but no information on the gas side can be obtained. Furthermore, temperature measurements are restricted to discrete points and thus cannot provide a detailed insight into the physical mechanisms which are important for an improved understanding of the unsteady engine wall heat transfer.

An early attempt to investigate the velocity boundary layer in ICEs by LDV was done by Foster et al. [76], who measured the velocity up to a distance of 60 $\mu m$ away from the wall. In this study two swirl levels with an engine speed of 300 $rpm$ were investigated, showing boundary layer thicknesses of less than 200 $\mu m$ for the high swirl and between 700 and 1000 $\mu m$ for the low swirl operating point. However, LDV can only measure the velocities in discrete points and hence drawing conclusions for the boundary layer in the whole engine is problematic.

During the past decade, LDV was gradually replaced by PIV which is able to provide instantaneous two- or three-dimensional velocity fields [28]. One of the first works studying the velocity boundary layer in ICEs by using PIV was published in 2010 by Alharbi et al. [77]. The investigated engine had a compression ratio of 9, a bore of 86 $mm$ and was operated with a turning speed of 800 $rpm$. The velocity boundary layer was observed on
2.3. Boundary layer and wall heat transfer

A planar slice at the cylinder head with a spatial extent of $2.25^2 \text{mm}^2$ and a minimum resolution of 45 $\mu\text{m}$. In addition, the velocities were measured on a larger slice with a size of $11.7 \times 9.7 \text{mm}^2$ and a spatial resolution of 343 $\mu\text{m}$. The results showed poor agreement with the law-of-the-wall and vortical structures were identified, which had a strong influence on the local velocity boundary layer. In 2013, the velocity boundary layer on the same engine at 400, 800, and 1100 rpm was studied by Jainski et al. [2]. Good agreement with the law-of-the-wall was found in the viscous sublayer ($y^+ < 5$), but large deviations were reported in the buffer and log law regions. The differences were attributed to discrepancies between the global ICE flow field and the steady flow in channel or pipe flows. The boundary layer thickness was found to decrease during the compression stroke and with higher turning speeds.

Due to the complex and variable geometry in internal combustion engines, to the best of our knowledge, no numerical studies which fully resolve the boundary layers in ICEs can be found in the literature. In contrast to this, the boundary layers of flow types like channel flows, pipe flows and stagnation flows are documented much better. Locally, the flow field at the ICE walls can be similar to those flow types. In some locations, the fluid flows mainly parallel to the wall (comparable to a channel flow) while in other regions the flow is directed towards the wall (comparable to a stagnation flow). Thus, in the following the findings of DNS investigations in channel and stagnation flows at conditions which are related to ICEs are summarized.
2. Literature review

One of the first incompressible and isothermal channel flow calculations using DNS was published by Kim et al. [78]. High order turbulence statistics were reported in order to provide reference data for the development of turbulence wall models. The results showed very good agreement with the law-of-the-wall and the experimentally derived data from Kreplin et al. [79].

Depending on the piston position in ICEs, the temperature at the wall can differ significantly from the temperature of the bulk gas. As a result, a thermal boundary layer is created, which in channel flows was found to have a similar structure as the velocity boundary layer when scaled by the Prandtl-number [80]. The influence of non-isothermal conditions on boundary layers was investigated by Huang et al. [81] in supersonic fully developed channel flows with fixed wall temperatures using DNS. For the transformation into non-dimensional wall units, in addition to the classical scaling \( y^+ = \frac{y}{\nu_W} \sqrt{\frac{\tau_W}{\rho_W}} \), where \( y \) is the dimensional wall distance, \( \nu_W \) the kinematic viscosity at the wall, \( \rho_W \) the density at the wall and \( \tau_W \) the wall shear stress) a density-based scaling (semi-local scaling) was proposed. With the use of the semi-local scaling a collapse of near wall shear stresses, turbulent kinetic energy and turbulent heat flux was reported in the two performed simulations, indicating that the differences to incompressible cases are mainly attributed to density variations. In the studies of Nicoud [82,83], boundary layers in channel flows with relatively low flow velocities and large temperature gradients were investigated using DNS. Compared to Huang et al. [81], the conditions were more relevant to ICEs. The results supported the density-weighted scaling for mean velocity, mean temperature
and streamwise velocity fluctuations, but no overlap was found for the velocity fluctuations in the wall normal and spanwise directions.

In addition to the temperature gradients, the pressure in internal combustion engines is also changing dynamically, which due to the $dp/dt$ term in the energy equation affects the thermal boundary layer. Bradshaw and Huang [84] reviewed the law-of-the-wall under variable spatial pressure gradients based on experimental data. In contrast to the velocity boundary layer, the pressure gradients were shown to have a strong effect on the law-of-the-wall for the temperature.

In addition to varying thermodynamic conditions (variable temperature and pressure), the ICE flow field differs significantly from the steady flow in channel or pipe setups. The impact of complex three dimensional flows on the boundary layer was reviewed by Bradshaw and Huang [85]. It was concluded, that the law-of-the-wall does not adequately describe complex 3D boundary layers. The thermal law-of-the-wall was shown to be even more sensitive to the mean flow and can only be applied to relatively simple one-dimensional flows.

In the work of Hattori and Nagano [86] the thermal and velocity boundary layers were investigated in impinging jet setups using DNS. Three setups with different channel heights were simulated with a Reynolds number of 9120. At all observed locations thermal and velocity boundary layer showed significant deviations from the law-of-the-wall. The largest differences were observed close to the center of the impinging jet, where the mean flow was mainly directed normal to the wall. Furthermore the variation of the Nus-
2. Literature review

selt number with increasing distance from the impinging center indicated a strong influence of the wall normal velocity component on the local wall heat transfer. The numerical work of Hadziabdic and Hanjalic [87] provides detailed insights into the flow field, vortical and turbulence structures and their correlation with the local heat transfer for an impinging jet flow. The instantaneous velocity and temperature fields revealed interesting temporal and spatial dynamics of vorticity and eddy structures and their imprints on the target wall. The dominant mechanism governing the flow and heat transfer was found to be roll-up vortices, which were generated by instabilities in the shear layer of the incoming jet. These vortices impose secondary structures, which transport boundary layer gases away from the wall and hence were shown to have a significant influence on the local wall heat transfer.

Despite the advances, phenomena like the influence of the complex ICE flow field and the temporally varying pressure which results in a temporally-varying kinematic viscosity remain uninvestigated.

2.3.2 Modeling

Different models have been proposed in the literature for the calculation of the engine wall heat transfer ranging from 0D global to multidimensional models. An overview of the different model types can be found in the review of Borman and Nishiwaki [12]. All engine wall heat transfer modeling approaches face the same problem: experimental methods can only partially access the ICE near wall regions and hence fundamentally little is
known about velocity and thermal boundary layer [12]. Thus many physical processes concerning the ICE heat transfer are still not understood and according to Angelberger et al. [88] the predictive capabilities of the modeling approaches are very limited. In the following an overview of different wall models and their underlying assumptions is presented.

**Gobal wall models**

Global thermodynamic models work with overall empirical heat transfer coefficients, which are assumed to be constant for all surfaces of the cylinder. This model type is mainly used for the thermodynamic analysis of experimentally derived in-cylinder pressure traces. Widely used global models were proposed by Woschni [5] and Hohenberg [6], who developed empirical correlation functions, to estimate the global heat transfer coefficient based on temperature, pressure and the engine geometry/kinematics. The heat transfer during compression, assuming a non-swirling case, is calculated according to Woschni by:

\[
\alpha_W = 3.26 d^{-0.2} \times p^{0.8} \times T^{-0.55} \times (2.28 s_p)^{0.8}
\]  

and according to Hohenberg by:

\[
\alpha_H = 130 V^{-0.06} \times p^{0.8} \times T^{-0.53} \times \left( T^{0.163} (s_p + 1.4) \right)^{0.8}
\]  

where \(d\) is the cylinder diameter, \(V\) the cylinder volume, \(p\) the average pressure, \(T\) the average temperature and \(s_p\) the mean piston speed.

Chang et al. [89] investigated the wall heat transfer in HCCI engines
based on instantaneous wall temperature measurements and compared the results with the global models from Woschni and Hohenberg. The results showed that the original Woschni model does not agree with the thermocouple measurements. In contrast to this, the model of Hohenberg gave better predictions, but had difficulties tracking the effects of load variation.

**Wall models for 3D engine simulations**

Three-dimensional RANS and LES engine simulations also depend on wall models for the simulation of wall heat transfer, since the mesh resolutions at the walls are too coarse to resolve the high velocity and temperature gradients close to the wall. The wall boundary layers are commonly modeled based on the wall function approach by Patanker and Spalding [90], which is based on the law-of-the-wall. Although the approach was initially developed for the boundary layer in steady, incompressible and fully-developed flows in smooth pipes/channels at moderate Reynolds-numbers, but it is also employed for other applications.

The flow and temperature field in ICEs violates several of the standard wall function assumptions. According to Nijeweme et al. [91] the main assumptions implicit in the standard wall-function treatment of Patanker and Spalding [90] are:

- steady flow;
- incompressible (i.e. no change in density);
- essentially one dimensional flow, such that gradients of velocity and scalar quantities are only normal to the wall;
2.3. Boundary layer and wall heat transfer

- small pressure gradients;
- the turbulence in local equilibrium;
- the turbulence length scale varies linearly with distance from the wall;

It is obvious that under realistic engine conditions many of these assumptions are violated. In order to reduce the modeling errors, Han and Reitz [92] improved the standard wall function approach for RANS models by taking gas density variations into account. Under the assumption of no chemical reactions the heat flux is then calculated as follows:

\[
q_{w,H} = \frac{\rho c_p \sqrt{\tau_W / \rho} T \ln(T/T_w)}{2.1 \ln(y^+) + 2.5}
\]  

(2.3)

where \( \rho \) is the density, \( c_p \) the heat capacity, \( \tau_W \) the wall shear stress, \( T \) the temperature, \( y^+ \) the wall distance in wall normal units and the numerical values 2.1 and 2.5 were derived based on fitting the experimental data of Kays [93]. The modeled heat transfer showed satisfactory agreement compared to experimental data in a premixed charged engine. In parallel, Angelberger [88] also improved the standard wall function approach for RANS models by considering the effect of temperature and thereby density gradients within the boundary layer. In addition, a model for simulating the influence of near wall flame quenching was developed. The calculated heat fluxes were compared to heat fluxes in a four-valve spark-ignited engine and found to be in reasonable agreement. However, the heat fluxes in the experiment were derived based on the global 0D heat transfer model from Woschni [5], which according to Chang et al. [89] showed significant
deviations to experiments at certain operation points. Nijeweme et al. \cite{91} discussed the law-of-the-wall assumptions for modeling heat transfer in ICEs based on the one-dimensional energy equation:

$$\rho c_p \frac{\partial T}{\partial t} + \rho v c_p \frac{\partial T}{\partial y} = \frac{\partial q_y}{\partial y} + \frac{dp}{dt}$$ (2.4)

where $y$ and $v$ point normal to the wall. Very important for the accurate description of wall heat transfer ($\frac{\partial q_y}{\partial y}$) was found to be the convection flow normal to the wall ($v$), which is formed due to density changes arising from both pressure and temperature changes in the boundary layer. In addition, the time-varying pressure term ($\frac{dp}{dt}$) was found to increase the wall heat transfer during compression and shift the heat flux peak towards earlier times. The wall heat transfer models by Han und Reitz \cite{92} and Angelberger et al. \cite{88} do not account for the convective flow due to density variations, since they still utilize a constant density approximation at one stage to complete the analytical wall function. The recent model of Keum et al. \cite{94} avoided the constant density approximation by tuning the model constants based on experimental data. In order to capture the effects of variable density within the boundary layer a non-dimensional temperature variable ($\Pi$) is introduced in the heat transfer equation (equation (2.3))

$$\Pi = \left( \frac{T_c}{T_w} \right)^M$$ (2.5)

where $T_c$ is the temperature of the first cell at the wall, $T_w$ is the wall temperature and $M$ is an empirical constant, which is derived in Park et
al. [95] by matching the heat release rate against the experimental data of Alkidas and Myers [96]. However, an evaluation of the model performance is difficult, since only comparisons with heat fluxes derived based on the standard wall function approach were reported.

Modeling of engine wall heat transfer using RANS faces a general drawback, since RANS solves only for the mean flow field, while the information for the instantaneous flow field is crucial for deriving the local heat flux distribution at the walls. In addition, the modeled turbulent kinetic energy is per construction isotropic, which disagrees with the strongly non-isotropic turbulent structures close to the engine walls.

According to Rutland [53] wall models for LES engine simulations also are not well developed. The main problem is again the mesh resolution close to the walls, which is typically too coarse to resolve the steep velocity and thermal gradients in the boundary layers and wall function models are used in LES. The recent work of Plengsaard and Rutland [97] proposed an improved wall model by extending the model of Han and Reitz [92] to LES using the Werner-Wengle model [98]. The latter model calculates wall shear stresses by assuming that the instantaneous tangential velocity in the first near-wall cell is in phase with the wall shear stress. Based on this assumption an updated friction velocity can be calculated which is included in the heat flux equation (equation (2.3)). Compared to RANS, LES provided improved agreement with experimental heat flux data; nevertheless, significant deviations compared to the experiments remain. The recent work of Nuutinen et al. [99] further improved the wall function approach by accounting
for the effects of variable density, multicomponent property variations and convection. An imbalance wall function based on the work of Popovac and Hanjalic [100] was introduced, which takes departures of the flow field from wall parallel mean velocities into account. The model was validated against the strongly heated pipe flow investigated experimentally by Shehata and McEligot [101] and numerically via DNS by Bae et al. [102] and very good agreement was observed. In addition, model validation with results from the pancake engine also used by Angelberger et al. [88] showed improved agreement with the experimental data in comparison to [88]. However, it should be noted that the simulations of the pancake test engine are not comparable to real engine conditions, since temperature und velocity fields are homogeneously initialized at BDC.

In summary, all wall heat transfer modeling approaches face the same problem: the lack of fully resolved calculations accurately describing the boundary layer under engine relevant conditions. Global models have been found to be able to capture general trends but have difficulties tracking the effects of load and engine speed variations. The modeling of ICE wall boundary layers in RANS and LES is mainly based on the wall function approach, which has been improved to take into account the thermodynamic conditions in ICE. However, according to Alharbi et al. [77] and Jainski et al. [2] it is questionable if an approach based on the law-of-the-wall can accurately predict wall heat transfer in internal combustion engines.
Chapter 3

Numerical Approach

The governing equations, discretization method and solver used for the detailed numerical simulations are presented in sections 3.1 and 3.2, respectively. The implementation of the Arbitrary Langrangian-Eulerian (ALE) formulation and the variable pressure term are described and validated in sections 3.3.1 and 3.3.2.

3.1 Governing equations

For the numerical simulation of low speed compressible reacting flows the existence of acoustic pressure waves places a severe restriction on the integration time step, due to the large discrepancy between the flow velocity and the speed of sound. When acoustic waves are not of interest, regular perturbation techniques can be used to decouple the waves from the governing equations [103]. The formulation used in the thesis is similar to the asymptotic analysis of Majda and Sethian [104] who derived a low-Mach number model to filter out acoustic waves. This analysis leads to a decomposition
of the pressure as,
\[ p(x,t) = p_0(t) + \varepsilon p_1(x,t), \tag{3.1} \]
where the hydrodynamic pressure \( p_1 \) is decoupled from the thermodynamic pressure \( p_0 \). \( \varepsilon \) is defined as \( \gamma Ma^2 \), where \( \gamma \) is the heat capacity and \( Ma \) the Mach number. The resulting low-Mach number governing equations for multicomponent reactive gaseous mixtures are:

**Continuity**
\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3.2}
\]

**Momentum**
\[
\rho \left( \frac{\partial \mathbf{v}}{\partial t} + \mathbf{v} \cdot \nabla \mathbf{v} \right) = -\nabla p_1 + \nabla \cdot (\mu \mathbf{S}) \tag{3.3}
\]
\[
\mathbf{S} = \nabla \mathbf{v} + (\nabla \mathbf{v})^T - \frac{2}{3} (\nabla \cdot \mathbf{v}) \mathbb{I} \tag{3.4}
\]

**Energy**
\[
\rho c_p \left( \frac{\partial T}{\partial t} + \mathbf{v} \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^{N_g} h_i \dot{\omega}_i \tag{3.5}
\]
\[
-\rho \left( \sum_{i=1}^{N_g} c_{p,i} Y_i \dot{V}_i \right) \cdot \nabla T + \frac{\gamma}{\gamma - 1} \frac{dp_0}{dt}
\]

**Gas-phase species**
\[
\rho \left( \frac{\partial Y_i}{\partial t} + \mathbf{v} \cdot \nabla Y_i \right) = -\nabla \cdot (\rho Y_i \dot{V}_i) + \dot{\omega}_i \quad i = 1, \ldots, N_g \tag{3.6}
\]
In equations (3.2) to (3.6) \( N_g \) is the total number of gaseous species, while \( h_i, \dot{\omega}_i, Y_i, \dot{V}_i, W_i, c_{p,i} \) are enthalpy, chemical production term, mass fraction,
3.1. Governing equations

diffusion velocity vector, molecular weight, and heat capacity of species \( i \), respectively. \( \lambda \) is the thermal conductivity, \( \mu \) the dynamic viscosity, \( \rho \) the density, \( \gamma \) the heat capacity ratio, \( c_p \) the heat capacity of the mixture and \( I \) is the identity matrix.

Assuming that the simulated gas mixture behaves ideally, the equation of state is an additional equation which couples pressure, density and temperature.

\[
p_0 = \rho \frac{RT}{\bar{W}} \quad (3.7)
\]

Here, \( \bar{W} = \left( \sum_{i=1}^{N_g} \frac{Y_i W_i}{\bar{W}_i} \right)^{-1} \) is the mean molecular weight of the mixture, and \( R \) the universal gas constant.

In the following the equations for calculating the flow field in section 4 will be described for the case of an open system for which \( p_0 \) is constant in time and thus \( \frac{dp_0}{dt} = 0 \). In section 3.3.2 the equations will be extended to describe temporally varying thermodynamic pressures, which is needed for the calculation of the compression stroke in section 5. In the context of low-Mach number combustion, the differentiated equation of state can be used to eliminate the density in the continuity equation (3.2). The resulting equation becomes:

\[
\nabla \cdot \mathbf{v} = -\frac{1}{\rho} \frac{DP}{Dt} = \frac{1}{T} \frac{DT}{Dt} + \bar{W} \sum_{i=1}^{N_g} \frac{1}{W_i} \frac{DY_i}{Dt} =: Q_t \quad (3.8)
\]

where \( Q_t \) is the thermal divergence. Equation (3.8) couples the temperature and species fields to the flow field. Furthermore, it shows that density is only determined by the thermodynamic state \( T, Y_i \) and \( p_0 \) and not by the
3. Numerical Approach

velocity, since acoustic waves are neglected. In contrast to this, incompressible formulations do not consider the effect of density variations, since $\nabla \cdot \nu$ is identically zero.

The diffusion velocities are calculated based on the Hirschfelder-Curtiss approximation [105]. The model accounts for the first term in the convergent series expansion and is the best first-order approximation to the full matrix diffusion as shown in Giovangigli [106]. After neglecting Soret and Dufour effects, the diffusion velocity $\tilde{V}_i$ for species $i$ becomes:

$$\tilde{V}_i = -(D_i/X_i) \nabla X_i, \quad D_i = \frac{1 - Y_i}{\sum_{j \neq i} X_j/D_{ji}},$$

with $D_{ji}$, $D_i$ and $X_i$ being species binary diffusion coefficients, mixture-averaged diffusivity and mole fraction for each species $i$, respectively. In order to ensure that despite the simplifying assumptions the mass fraction weighted sum of the diffusion velocities is equal to zero as required by mass conservation, the correction velocity

$$V_i = \tilde{V}_i + V_c, \quad V_c = -\sum_{i=1}^{N_g} Y_i \tilde{V}_i$$

needs to be introduced [107].

The reaction rate constants for the calculation of chemical source terms ($\dot{\omega}_i$) in equations (3.5) and (3.6) are assumed to follow an extended Arrhenius expression. In this work no chemical reactions are considered and therefore the chemical source term $\sum_{i=1}^{N_g} h_i \dot{\omega}_i$ in equation (3.5) is always zero.
3.2 Solver and numerical method

Finite and spectral element methods are applications of the method of weighted residuals. In this technique trial functions are employed as basis functions for a truncated series expansion of the solution of the partial differential equations. The residual error resulting from the substitution of the approximate solution in the partial differential equations is minimized by introducing test or weighting functions. The choice of the expansion and the test function defines the type of discretization method (e.g. finite or spectral element method) [108]. In case of spectral-Galerkin methods trial and test functions are chosen to be the same and are taken to be $N^{th}$-order tensor product polynomials based on the Gauss quadrature points determined by the roots of orthogonal polynomials. The method yields exponentially convergent dispersion errors and features excellent transport properties (minimal numerical diffusion and dispersion) for a significantly larger fraction of the resolved modes compared to higher order finite difference and finite volume methods. [109]

The spectral element method (SEM) combines the advantages of spectral-Galerkin methods with those of finite element methods due to the application of the spectral method per element. Thus, the tensor product efficiency of global spectral methods is combined with the geometric flexibility of finite element methods. In this work the SEM proposed by Patera et al. [110] is used for the discretization of the equations reported in section 3.1. This is done by first splitting the domain into $E$ hexahedral elements and then dividing each element $E$ by polynomials with the order $N$ in the spatial
3. Numerical Approach

The simulations were carried out using the open source spectral element flow solver Nek5000 [17], a Computational Fluid Dynamics (CFD) solver based on the spectral element method developed at Mathematics and Computer Science Division of Argonne National Laboratory. The code is written in Fortran 77 and C and the MPI standard is used for parallelization. It is specially tuned for a high parallel efficiency and at maximum a linear scaling of up to 524,288 processors is reported in [17]. Additional information’s about Nek5000 can be found on the official homepage [17].

The equations in section 3.1 are solved by the high-order splitting scheme for low-Mach number reactive flows described in Tomboulides et al. [4]. A schematic of the solution algorithm is shown in figure 3.1, where due to the low Mach number formulation the thermo-chemistry subsystem...
can decoupled from the hydrodynamic subsystem. This has the advantage, that an appropriate stiff ordinary differential equation solver can be used to solve the discretized partial differential equations for energy and species in a fully-coupled way, avoiding additional splitting errors. In the thermo-dynamic subsystem the spatially discretized energy and species equations yield a system of ordinary differential equations (ODE), which in time is integrated with the variable $q^{th}$-order ($q = 1, ..., 5$), variable-step integrator CVODE [111]. The density has been removed from the equations by using the equation of state. The equations are solved implicitly with the exception of the velocities which are calculated based on a high-order explicit extrapolation scheme. The link between thermo- and hydrodynamic subsystem are the density and the divergence constraint ($Q_t = \nabla \cdot v$), which accounts for the influence of density variations on the velocity field. The solution of the hydrodynamic subsystem is based on a projection type velocity correction scheme introduced by Orszag et al. [112]. Using a splitting scheme in a first step a pressure Poisson equation is solved using a 3rd-order extrapolation scheme for velocities in the viscous term. Once the hydrodynamic pressure $p_1$ is known the velocity is corrected in a second implicit viscous correction step based on standard Helmholtz equations. The low Mach number formulation features a high time accuracy for all hydrodynamic variables in combination with minimal splitting errors as shown in Tomboulides et al. [4] and Orszag et al. [112].
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3.3 Code extension

Nek5000 features the implementation of the Arbitrary Lagrangian-Eulerian (ALE) formulation of Ho [20,113], which employs polynomial orders for the solution of the velocity (polynomial order n) and pressure (polynomial order n-2) fields [109]. The so-called P\textsubscript{n}-P\textsubscript{n-2} formulation was modified for the purposes of this thesis for a formulation where the same mesh is employed for both variables (P\textsubscript{n}-P\textsubscript{n} formulation [4]) as described in sub-section 3.3.1. In subsection 3.3.2 the code modifications for calculating variable thermodynamic pressures are discussed. Code development was done in collaboration with Professor Ananias Tomboulides from the University of Western Macedonia, Greece.

3.3.1 Arbitrary Langrangian-Eulerian (ALE) formulation

In this work, the ALE method is used to account for moving geometries. A large advantage of the ALE method is that the computational domain can deform independently from the fluid motion, which allows for arbitrary mesh movement within the limits of mesh distortion. Compared to the Eulerian form (equation (3.3)) the mesh velocity \( w \) is introduced in the convective term and the temporal derivative of the velocity \( \frac{\partial u}{\partial t} \) is relative to the ALE coordinate system and not to a fixed Eulerian coordinate system. Thus equation (3.3) becomes:

\[
\rho \left( \frac{\partial v}{\partial t} + (v - w) \cdot \nabla v \right) = -\nabla p_1 + \nabla \cdot (\mu \mathbf{S}) \tag{3.11}
\]
Similar to the momentum equation, the ALE form of temperature and species equations are derived by introducing the mesh velocity \( \mathbf{w} \) in the convective operator in equations (3.5) and (3.6), which become:

**Energy**

\[
\rho c_p \left( \frac{\partial T}{\partial t} + (\mathbf{v} - \mathbf{w}) \cdot \nabla T \right) = \nabla \cdot (\lambda \nabla T) - \sum_{i=1}^{N_g} h_i \dot{\omega}_i - \rho \left( \sum_{i=1}^{N_g} c_{p,i} Y_i \mathbf{V}_i \right) \cdot \nabla T + \gamma \frac{\gamma - 1}{\gamma} \frac{dp_0}{dt} \quad (3.12)
\]

**Gas-phase species**

\[
\rho \left( \frac{\partial Y_i}{\partial t} + (\mathbf{v} - \mathbf{w}) \cdot \nabla Y_i \right) = -\nabla \cdot (\rho Y_i \mathbf{V}_i) + \dot{\omega}_i \quad i = 1, ..., N_g \quad (3.13)
\]

A detailed derivation of the ALE-equations can be found in Donea et al. [114].

The ALE formulation in this work extends the existing P\(_n\)-P\(_{n-2}\) ALE-formulation to the P\(_n\)-P\(_n\) approach. For the implementation into Nek5000, equation (3.11) was transformed into its weak form:

\[
\frac{d}{dt} \int_V \rho \varphi \cdot \mathbf{v} \, dV = -\int_V \rho \varphi \cdot (\mathbf{v} \cdot \nabla \mathbf{v} - \nabla \cdot \mathbf{v} \mathbf{w}) \, dV + \int_V \varphi \cdot \nabla p \, dV - \int_V \mu \nabla \varphi \cdot \nabla \mathbf{v} \, dV \quad (3.14)
\]

where \( \varphi \) is the test function and \( V \) the domain volume. The boundary integral terms are neglected since in this work only Dirichlet boundary conditions are used. The ALE formulation was implemented by adding the
additional term $\nabla \cdot \bar{v} \bar{w}$ into the momentum equation. The ALE approach in the energy and species equations is implemented into Nek5000 by replacing the fluid velocity ($\bar{v}$) in the convective term by ($\bar{v} - \bar{w}$).

**Validation**

The discretization scheme of the convective term including the mesh velocity used in the newly implemented ALE method in the $P_n$-$P_n$ formulation is identical to the one used in the $P_n$-$P_{n-2}$ approach by Ho and Patera, which was extensively validated in [20, 113]. Furthermore the accuracy of this scheme was also assessed by Bjontegaard and Ronquist [115] using an analytic solution in an expanding mesh setup. The mesh expands in one spatial direction and thus is very similar to mesh motion of the present study in section 4.

The $P_n$-$P_n$ implementation of the ALE approach is validated by comparison with the $P_n$-$P_{n-2}$ implementation in a peristaltic moving 3D-tube setup shown in figure 3.2. The setup has been chosen, since the moving mesh strongly influences the temporal and spatial evolution of the velocity field. The pipe has initially a non-dimensional diameter of $d = 1$ and a length of $L = 16$. Due to the imposed mesh velocity the pipe thickness is changing continuously, resulting in a peristaltic pumping movement. The
imposed mesh velocity is:

\[
\begin{align*}
    w_x &= -0.5 (\varepsilon_z \ast \varepsilon_t) 2x \cos(\left(\frac{1}{3} \pi z\right) - t) \\
    w_y &= -0.5 (\varepsilon_z \ast \varepsilon_t) 2y \cos(\left(\frac{1}{3} \pi z\right) - t) \\
    w_z &= 0
\end{align*}
\]

where \( \varepsilon_z = \frac{\sinh(0.2z)}{\cosh(0.2z)} \) and \( \varepsilon_t = \frac{\sinh(0.2t)}{\cosh(0.2t)} \). The Reynolds-number is always below 200 so that the flow remains laminar. At the inflow a steady parabolic velocity profile with a maximum axial velocity \( v_z \) equal to 1 at the cylinder center is imposed while at the outflow zero-Neumann boundary conditions are used. At the pipe walls the velocity is set equal to the mesh velocity in order to prevent a flow across the walls. The numerical setup including the mesh is included in the example peris of the Nek5000 package \[17\].

Figure 3.2 shows the velocity magnitude \( |v| \) distribution on an axial slice through the pipe. The highest flow velocities can be observed in regions with larger pipe diameters. The velocity magnitude of the \( P_n-P_n \) ALE formulation implemented in this work is compared to the \( P_n-P_{n-2} \) im-
3. **Numerical Approach**

Figure 3.3: Comparison of the instantaneous and the averaged axial velocity magnitude between the $P_n-P_{n-2}$ and the $P_n-P_n$ approaches at $t = 50$.

The implementation at $t = 50$ in figure 3.3. The dashed line and the circle markers represent the axially averaged velocity magnitude versus the channel length, while the solid line and the square markers indicate the velocity magnitude along the centerline (marked by the dashed line in figure 3.2). The mean and the instantaneous velocity magnitudes show an excellent agreement between the two formulations.

The implementation of the ALE approach in the temperature equation is validated by simulating in the same setup using non-isothermal conditions at the inflow. Initial and boundary conditions for the velocity field and mesh movement are identical to the previously described flow validation case. The temperature at the walls is fixed to $T/T_{ref} = 1$, where $T_{ref} = 300K$. At the inflow a parabolic temperature profile is imposed with a maximum temperature of $T/T_{ref} = 1.125$ in the pipe center while zero-Neumann boundary conditions are used at the outflow boundary. A homogeneous $N_2/O_2$ mix-
3.3. Code extension

Figure 3.4: Comparison of the temperature fields on a x-z slice between the ALE approaches for the $P_n-P_{n-2}$ and the $P_n-P_n$ formulation at $t = 8$.

The computed temperature fields are illustrated at $t = 8$ in figure 3.4. The decreasing temperatures in the flow direction are due to the cooler pipe walls. The local temperature peaks in the thicker pipe segments due to the higher distance from the cylinder wall. Figure 3.4 shows the very good agreement of the temperature fields obtained using the two formulations, as also seen in the instantaneous temperatures along the centerline (figure 3.5).

3.3.2 Variable pressure term

During the compression stroke in section 5 the system is no longer open, which leads to a temporal varying thermodynamic pressure ($\frac{dp}{dt} \neq 0$). Thus, for the solution of the thermodynamic subsystem it is necessary to compute...
3. Numerical Approach

Figure 3.5: Comparison of the instantaneous centerline temperatures between the ALE approaches for the $P_n-P_{n-2}$ and the $P_n-P_n$ approach at $t = 8$.

The temporal pressure gradient $\frac{\partial p_0}{\partial t}$. Equation (3.8) then becomes:

$$\nabla \cdot \mathbf{v} = \frac{1}{T} \frac{DT}{Dt} + \overline{W} \sum_{i=1}^{N_p} \frac{1}{W_i} \frac{DY_i}{Dt} - \frac{1}{p_0} \frac{dp_0}{dt} =$$

$$= Q_t + \frac{1}{p_0} \frac{dp_0}{dt} \left( -1 + \frac{\gamma}{\gamma - 1} \frac{R}{W_{cp}} \right)$$

(3.15)

where $Q_t$ is the thermal divergence assuming a constant hydrodynamic pressure (equation (3.8)). After rearranging and integrating over the domain the temporal pressure gradient is calculated as follows:

$$\frac{dp_0}{dt} = \frac{p_0}{\sum \left( 1 - \frac{\gamma}{\gamma - 1} \frac{R}{W_{cp}} \right)} \left( \sum Q_t - \sum dV \right)$$

(3.16)
where $dV$ is the change of the volume, the mean specific heat is $c_p = \sum_{i=1}^{N_g} c_{p,i} Y_i$ and the $\sum$ operator stands for the sum over all nodes. The detailed derivation of equation (3.16) can be found in Daru et al. [116].

**Validation**

The implementation of the variable thermodynamic pressure is validated by comparison with a zero dimensional CHEMKIN simulation for an isentropic compression case. A two dimensional setup with a constant width of 75 mm and an initial height of 90 mm is compressed until a height of 15 mm is reached. This results in a compression ratio of 6 and the piston speed is 200 rpm. Homogeneous condition for temperature ($T = 819.45$ K), pressure ($p = 1$ atm) and composition ($Y_{N_2} = 0.7288$, $Y_{O_2} = 0.1937$ and $Y_{CH_4} = 0.0775$) are used at BDC. Zero velocity boundary conditions are employed at the liner and the cylinder head and the piston velocity is imposed at the piston. Zero flux conditions are imposed for the temperature and species boundaries at all walls. For the 0D homogeneous adiabatic CHEMKIN [117] calculation the same geometry and initial conditions are considered. The chemical reactions are in both cases calculated based on a reduced mechanism for CH$_4$ combustion with 21 species and 87 reactions.

In figure 3.6 the computed temperature and pressure time histories are compared with the 0D - CHEMKIN calculation. At time $= 0$ the piston is at BDC and at $t = 4$ at TDC. The continuously increasing temperature during compression, results in auto-ignition at a non-dimensional time $t \approx 3$. At TDC the temperature and pressure are 2731 K and 20 atm, respectively. Both figures show nearly identical evolutions of the temperature and pres-
3. Numerical Approach

![Comparison of temperature and pressure evolution](image)

Figure 3.6: Comparison of the temperature (a) and pressure (b) evolution during compression between CHEMKIN and Nek5000.

sure profiles. The minimal offset in the auto-ignition timing lies within the uncertainty of numerical settings like the chosen time steps or the imposed tolerances. The author likes to thank Mahdi Kooshkbaghi for providing the reduced chemistry mechanism and his help in the 0D CHEMKIN calculation.
Chapter 4

DNS of multiple cycles in an engine-like geometry

4.1 Introduction

In this section multiple cycles in an engine-like geometry are investigated. The experimental and numerical setup are described in sections 4.2 and 4.3. In the results section first the influence of the grid resolution is assessed in section 4.4.1 and compared with experimental data in section 4.4.2. After that section 4.4.3 investigates the evolution of the flow field followed by its statistically analysis in section 4.4.4. The last part in this chapter (section 4.4.5) focuses on the investigation of the cause-and-effect relationships of the observed cycle to cycle variations of the flow field in the simulated setup. The presented material in this chapter appears in Schmitt et al. [118,119].
4. DNS of multiple Cylces in an Engine-like geometry

4.2 Geometry and experimental data

Simulations are performed in the axis-symmetric piston-cylinder assembly investigated experimentally by [21] shown schematically in figure 4.1(a). The piston kinematics are governed by a crankshaft turning at a constant speed of 200 rpm, which is sufficiently high to ensure turbulent flow within the cylinder. Through the fixed valve, the system is open to the environment so that compressibility is negligible. The assembly has a diameter (bore) of $D_c = 75$ mm, stroke $S = 60$ mm, and the clearance height between the flat piston and the cylinder head increases from 30 mm at Top Dead Center (TDC) to 90 mm at Bottom Dead Center (BDC). The valve angle is 30° with respect to the cylinder axis and the width of the uniform valve gap is 4 mm. The piston has a mean speed of $V_p=0.4$ m/s and reaches its maximum speed of approximately $V_{p,max}=0.63$ m/s at 90 and 270 crank angle degrees (°CA), while the maximum mean velocity of the inflowing jet is approximately 9.35 (the piston-to-valve-gap area ratio) times larger than $V_{p,max}$. The experiments were carried out with air at environmental conditions (1 atm and 293 K).

Laser-Doppler anemometry was used to measure the axial and azimuthal velocity components at 36°, 90° 144°CA during the intake stroke and at 270°CA during the exhaust stroke at points on planes located at intervals of 10 mm below the cylinder head in the axial direction and 5 mm in the radial direction. The mean and rms of axial the velocity were obtained by averaging over 100 samples within a 10°CA interval and five independent sets of measurements were taken to check the reproducibility.
4.3 Numerical setup

The 3-D geometry is discretized using 168,564 conforming hexahedral spectral elements matching the domain boundaries, which for the employed polynomial order of $n = 7$ results in 57.8 million discretization points. A
view of the spectral element skeleton constructed in a block-structured fashion to allow for local grid adaptation using the meshing software Cubit [19] is shown in figure 4.1(b). Since the volume ratio between TDC and BDC is three, no mesh layers need to be added during expansion and the number of elements remains constant during the simulation. In the central part, unstructured hexahedral elements are used to reduce the number of elements compared to an H-grid approach. In the channel above the valve two intermediate blocks are introduced to reduce the number of radial cells from the large radius at the outer wall to the small radius at the valve shaft.

The imposed mesh velocity \( w \) is always zero in the radial and azimuthal directions. In the axial direction \( w \) is zero in the clearance volume \((z > -10 \, mm)\). For \( z < -10 \, mm \), \( w \) increases linearly towards the piston, which moves with a velocity determined by the piston kinematics. It can be shown that for this particular linear variation of the mesh velocity in the axial direction which is used here, the GCL is exactly satisfied because of the fact that the divergence of mesh velocity, \( \nabla \cdot w \), is constant in space and is only a function of time. Furthermore, the elements angles are not distorted during the simulation, since the mesh movement is restricted only to the axial direction.

The mesh in the valve gap contains eight elements, which for the chosen polynomial order results in a spatial resolution of about 0.07 \( mm \). In the cylinder, the distance of the first point from the walls is 0.06 \( mm \), and the average resolution is approximately 0.1 \( mm \) in the radial and vertical direction and better than 0.2 \( mm \) in the azimuthal direction. Not shown
in figure 4.1(b) is the axis-symmetric large upper plenum, which is used in order to impose the inlet conditions far from the valve inlet. It has a cylindrical shape with a diameter of 112.5 mm and a height of 75 mm resulting in a volume of slightly larger than 2.8 times the displaced volume in the cylinder. The time-varying inflow velocity at the top of the plenum is uniform and determined by the instantaneous piston speed and the ratio of the plenum inflow and piston areas. No-slip boundary conditions are imposed along stationary walls.

The simulation is initialized with a quiescent velocity field with the piston positioned at TDC, and the conservation equations are integrated in time using the third-order mixed implicit-explicit scheme. In space the chosen polynomial order results in a discretization order of at least 7 \[109\]. The Reynolds number peaks at the time of maximum piston speed with \(Re_{\text{max}} = V_{p,\text{max}} D_c/\nu = 3070\). The time step is adjusted during the simulation in order to respect a fixed maximum Courant number of 0.45. In total, eight cycles are computed at a cost of approximately 160,000 CPUh per expansion-compression cycle on a CRAY XE6 system, resulting in a total computational time of 1.3 million CPUh.

With the exception of the radial distance which in the following will be normalized by the cylinder radius, the results are presented in dimensional form.

**Averaging and notation**

For stationary flows, statistical quantities are usually computed by averaging in time \[120\]. For non-stationary flows like the ones encountered in
time-varying geometries, ensemble-averaging should be used instead. This results in significantly higher computational cost since a sufficient number of cycles must be simulated in order to obtain converged statistics. Taking advantage of the axis-symmetric geometry considered here, a combination of azimuthal and ensemble averaging, referred to as total averaging henceforth, is used to reduce the number of required cycles. In total, eight cycles are calculated from which the first two are discarded from the statistical analysis in order to minimize the effect of the initial conditions. The same averaging approach was used in the LES of [46], where five cycles were simulated. The convergence of the statistics is described in section A.1 in the appendix.

In the following, for any variable $\psi$ its azimuthal average will be denoted as $\langle \psi \rangle_\varphi$, volume average in the cylinder as $\langle \psi \rangle_V$, ensemble average as $\langle \psi \rangle$, average over a plane at a fixed axial position $z$ below the cylinder head as $\langle \psi \rangle_z$, the total (azimuthal and ensemble) average as $\overline{\psi}$, while the velocity magnitude will be denoted as $|v|$. The locations where data is extracted on horizontal planes at a distance $p$ mm below the cylinder head will be referred to as $z_p$. Finally, the kinetic energy is $K = \frac{1}{2} \left( v_r^2 + v_\varphi^2 + v_z^2 \right)$ and the turbulent kinetic energy $k$ is defined as $k = \frac{1}{2} \left( v_r'^2 + v_\varphi'^2 + v_z'^2 \right)$, where $v_r'$, $v_\varphi'$ and $v_z'$ are the fluctuation velocity components in the radial, azimuthal and axial direction, respectively.
4.4 Results and discussion

4.4.1 Grid resolution study

The resolution requirements, which differ significantly as the flow evolves, are assessed at the highest $Re$ reached at the time of the maximum piston speed ($90^\circ$CA), by comparing the results of the same expansion stroke calculated in a new mesh with 266,186 elements and polynomial orders of 3, 5 and 7, resulting in grids with 7.7, 33.4 and 91.5 million grid points, respectively. The initial conditions are obtained by spectral interpolation of the flow at TDC of the third cycle computed using the 57.8 million nodes grid and $180^\circ$CA are simulated. Figure 4.2 shows the autocorrelation of the vorticity magnitude at $90^\circ$CA and at a location in the region with the highest rms velocities ($r = 33.75$ mm and $z = 18.75$ mm below the cylinder head). The autocorrelation of the vorticity magnitude depends strongly on the resolved turbulent scales and is therefore a good indicator for the mesh resolution. For the coarsest mesh the slope of the curve is significantly lower than the rest of the investigated resolutions, while for the 33.4 million cells mesh, the gradient is close to the two finer meshes. The two finer meshes show nearly identical slopes, indicating that the resolved turbulent length scales in both meshes are comparable.

The effect of the resolution on the mean and rms velocities normalized by the mean piston speed $\bar{V}_p = 0.4$ m/s is shown in figure 4.3. The comparison of the axial velocity component at $90^\circ$CA after TDC at $z = 10, 20, 30, 40$ and 50 mm below the cylinder head, and the mean and rms velocity
4. DNS of multiple cycles in an engine-like geometry

Figure 4.2: Autocorrelation of the vorticity magnitude at 90°CA at a radius of 33.75 mm and a height of 18.75 mm below the cylinder head.

profiles are computed using azimuthal averaging during a single expansion stroke. For the coarsest mesh, significant differences can be observed for the mean profiles at locations $z_{10}$ and $z_{20}$ and for the fluctuation profiles at all locations. The results obtained using the 33.4 million nodes grid show small differences at the location of maximum speed at $z_{10}$ for both the mean and rms values, while very similar results are obtained for the two finer meshes. Based on these results, the 57.8 million node grid is employed in the simulations.

4.4.2 Comparison between simulation and experiment

All the results presented in this section are obtained by azimuthal and ensemble averaging of the data for cycles 3 to 8. Comparisons with the experiments at 36°, 90°, 144°CA (intake stroke) and 270°CA (exhaust stroke) are shown in figure 4.4 for the streamlines and in figures 4.5-4.7 for the mean and rms of the axial velocity. The experimental data [21] were reported
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Figure 4.3: Comparison of the axial (a) mean and (b) rms velocities computed with different resolutions at 90°CA (azimuthal averaging over a single cycle is used).

(a) 36°CA  (b) 90°CA  (c) 144°CA  (d) 270°CA

Figure 4.4: Pseudocolor plot of the calculated mean velocity magnitude overlaid with streamlines (left subfigure) and experimentally determined isocontours of the streamfunction (right subfigure) at 36°, 90°, 144°CA and 270°CA.
in terms of iso-contours of the stream-function $\psi$ computed from the mean velocity $\overline{U}$ as a function of the crank angle $\theta$, $\partial \psi / \partial t = \rho \overline{U}(\theta) r$.

The mean flow is dominated by the hollow jet entering at an angle and with varying inflow velocity into the cylinder during the intake stroke, and by its interaction with the flow in the cylinder and the domain boundaries. Two vortex rings are formed initially, one in the region close to the symmetry axis and another near the corner of the cylinder head and cylinder liner (figure 4.4(a)). The two rings are initially of similar size, but as the piston moves downwards, the central clockwise rotating vortex grows in size to fill most of the cylinder. At 90\(^\circ\)CA, the jet has already impinged on the cylinder wall and has been deflected towards the piston, forming a third vortex ring at the corner of the piston with the cylinder wall (figure 4.4(b)). The third and the central vortex rings grow larger as the piston continues its downward motion (figure 4.4(c)). During the exhaust stroke the mean flow becomes essentially one-dimensional (figure 4.4(d)). Good agreement can be observed between experiments and simulation with respect to the flow features: the position and direction of the incoming jet, the axial position of the broadening of the jet streamlines and the position and sizes of the recirculation zones.

The total mean, $\overline{v_z}$, and rms, $(\overline{v_z'^2})^{0.5}$, of the axial velocity component extracted from the DNS data by azimuthal and ensemble averaging are compared with the experimental data in figures 4.5, 4.6 and 4.7 at 36\(^\circ\), 90\(^\circ\) and 144\(^\circ\)CA, respectively, on different planes below the cylinder head.

In good agreement with the experiment, the flow at 36\(^\circ\)CA is mainly
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Figure 4.5: Comparison of the mean and rms z-velocity between experiment and DNS data at 36°CA at different axial locations below the cylinder head (solid line: DNS, symbols: experiment).

drawn in the axial direction and the jet velocity is almost ten and five times the mean piston speed at 10 (z10) and 20 mm (z20) below the cylinder head, respectively, with the radial location of the maximum values remaining unaffected by the distance. Near the piston, the mean profile is practically flat and the velocity is close to $V_p$. The rms velocity profiles, which may also be interpreted as turbulence level, show that turbulence is generated in the shear layers between the incoming jet and the fluid side in the cylinder. The computed rms velocity peak at $z_{20}$ is about 30% higher than the measured value. This may be due to the high sensitivity of the rms values to the measurement location and time at $z_{20}$ as discussed below.

Following jet deflection at 90°CA, the peak values of the velocity shift towards the cylinder wall before the axial velocity profiles flatten for $z<40$ mm. Compared to the experiment, the simulation shows higher mean velocity magnitudes for $r > 0.8R_c$ at $z_{30}$ and $z_{40}$. The agreement improves later in
Figure 4.6: Comparison of the mean and rms z-velocity between experimental and DNS data at 90°CA at different axial locations below the cylinder head (solid line: DNS, symbols: experiment).

the cycle (144°CA, figure 4.7). As discussed in detail below, the cyclic variability of the mean velocity field at 144°CA is significantly lower compared to 36° and 90°CA, in agreement with the experimental observations [21].

It is worth pointing out that good agreement for all experimentally reported piston positions and profiles could only be obtained by including the last six simulated cycles. Azimuthal averaging of the single-cycle data resulted in good agreement only for some piston positions.

The LES results reported in [45] and [46] show good agreement with the experimental and the DNS data at 36° and 144°CA. However, at 90°CA the axial velocities at the cylinder wall is over predicted compared to the DNS and the experimental data. Based on the DNS results two reasons for
this discrepancy can be identified. First, the flow field at 90°CA is sensitive to the jet breakup process where the laminar jet flow becomes turbulent and is not easy to capture by LES simulations. In addition, as will be shown below, the DNS data indicate strong shear stresses in combination with small integral length scales in the shear layers of the incoming jet at 90°, indicating that higher resolution should be used in LES calculations in order to resolve the shear stress. The determination and values of the integral length scale will be discussed in section 4.4.4.

Figure 4.7: Comparison of the mean and rms \( z \)-velocity between experiment and DNS data at 144°CA at different axial locations below the cylinder head (solid line: DNS, symbols: experiment).
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4.4.3 Flow field

The flow dynamics are found to differ substantially from cycle to cycle. Instantaneous flow fields and the effect of the flow field at the end of one cycle to the flow dynamics in the subsequent cycle are discussed in this section. Particular attention is paid on the jet flow and the vortex ring formation during the intake stroke of the individual cycles.

4.4.3.1 Instantaneous flow fields

Pseudocolor plots of the instantaneous velocity magnitude during the expansion stroke of the first and third cycle on the $x-z$ plane are reported in figures 4.8(a) and (b). In the first cycle, the hollow jet created at the valve enters into the quiescent fluid in the cylinder. The highest velocities reached in the valve channel can be estimated by the piston speed and the area ratio of the piston to valve gap. Based on the maximum mean velocity in the valve channel of 5.9 m/s and the valve gap of 4 mm, the Reynolds number of the flow in the valve channel never exceeds $Re = 1531.2$ so that the flow remains laminar as discussed in section 4.4.3.2. When the fluid enters the valve channel, small recirculation zones are formed at the sharp edges at the inner and outer channel walls (a more detailed description of the flow in the valve channel is given in section 4.4.3.2). Up to 45°CA, the hollow cone jet displays no signs of instability. As it was also observed in the flow from inclined nozzles in [121], the roll up of the thin vorticity layers close to the channel walls at the valve exit results in the formation of a vortex ring pair on the sides of the hollow jet. The stronger inner vortex ring
close to the piston which is clearly visible at 45°CA, deflects the jet towards the axis before its impingement on the piston and its subsequent reflection towards the cylinder head. At 77°CA, Kelvin-Helmholtz instabilities are visible on the shear layers of the jet, which is deflected by the flow in the radial direction towards the cylinder walls. The interaction of the jet which attains highest momentum at 90°CA with other flow structures results in a turbulent flow field characterized by the large coherent structures enclosed by the vortex ring as well as a large number of small vortical structures. The instantaneous flow field at 135°CA (figure 4.8(a)) appears similar to that at 90°CA, but with a significantly lower jet velocity due to the reduced piston speed. During the exhaust stroke (not shown), the flow field loses most of its features as the fluid is pushed out of the cylinder by the upward piston motion.

These structures can be more clearly seen in the volume renderings of the vorticity magnitude reported in figure 4.8(c). At 36°CA, a large inner and a smaller outer vortex ring can be seen on either side of the laminar jet, which are connected to the vorticity layers in the valve channel; in the valve channel, $Re \approx 900$ and no instabilities can be observed. At 51.5°CA, the jet has already impinged on the piston and the inner ring has been deflected towards the cylinder head. Another vortex ring close to the piston is moving towards the cylinder wall while smaller rings can be seen on the shear layers of the incoming jet. At later times, the interaction of the large vortical structures with the incoming jet indicated by the arrows at 72°CA, results in splitting the jet into two large zones, one towards the cylinder center
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Figure 4.8: Instantaneous velocity magnitude in a cross section through the cylinder axis at different times during the expansion of the (a) first cycle and (b) the third cycle; (c) volume renderings of the instantaneous vorticity magnitude at different times during the expansion of the first cycle.
Figure 4.9: Instantaneous vorticity magnitude on a slice through the cylinder axis at different times during the expansion of the third and sixth cycle.

and a smaller one at the corner of the piston and cylinder wall. At point B, the small outer zone meets the incoming jet and creates small vortices towards the cylinder center. The inner recirculation influences the direction of the incoming jet, which at 90°CA is deflected to impinge directly at the cylinder wall (point C).

Due to the velocity field inside the cylinder at TDC of the previous cycle, the subsequent cycles are different. The comparison of the instantaneous velocity fields of the first and third cycles at 45°CA (figure 4.8(a) and (b)) shows that the vortex ring breaks up much earlier in the third cycle. The earlier transition to turbulence leads to increased dissipation which is responsible for the lower value of the velocity magnitude in cycle 3 at 90°CA (the volume integrated velocity magnitude values $\langle|v|\rangle_V$ are reported in table 4.1 and discussed below). At 135°CA the flow fields of
the first and third cycle look similar, although the higher velocity region is localized closer to the cylinder head for the former. The cyclic differences of the mean and fluctuation fields will be quantified below (figure 4.14).

Figure 4.9 reports the vorticity magnitude at different times during the expansion stroke of cycles 3 and 6. In contrast to cycle 1, the mean velocity and fluctuations at TDC of the previous cycle affect the incoming jet, which enters the cylinder in the presence of a cross-flowing stream. Instabilities at the tip of the incoming jet can be observed in both cycles already at 36°CA; the later evolutions however differ considerably: in cycle 3, the jet at 58.5°CA has impinged on the piston and formed the inner and outer recirculation zones indicated by the arrows, while in the sixth cycle the jet first impinges on the cylinder liner and the fluid flows along the wall, preventing the formation of an outer counter-clockwise rotating recirculation zone. At 76.5°CA the counter-clockwise rotating large scale structure of cycle 3 close to the piston supports the formation of a strong large flow structure below the valve rotating clockwise (figure 4.8). Due to the more wall-parallel flow of the sixth cycle, the large scale structure is elongated and less pronounced. As a result of these differences the subsequent flow field evolution varies considerably as will be described in the next sections. At 146°CA, an additional small vortex ring at the corner of the cylinder head with the wall forms in both cycles.
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4.4.3.2 Jet flow and vortex ring

Due to symmetry, the azimuthal velocity component of the incoming laminar jet is very small compared to the radial and axial velocities. With increasing piston speed after TDC the incoming jet accelerates and transition to turbulence occurs at the jet tip. At the transition location a strong increasing azimuthal velocity component can be observed, which is significant larger compared to the increase of $v_\varphi$ due to asymmetries in the large scale flow motions. In the following, the volumetric average of the azimuthal velocity $\langle v_\varphi^2 \rangle_V$ is used as quantitative indicator of the turbulent jet breakup process.

The time histories of $\langle v_\varphi^2 \rangle_V$ during cycles from two to eight are compared in figure 4.10(a). The values at 15°CA correspond to the fluctuation levels remaining at TDC of the previous cycle and correlate strongly with the velocity magnitude at TDC as will be shown in figure 4.17. Until 25°CA,
\( \langle v^2_\varphi \rangle_V \) remains almost constant for all cycles, and the incoming jet is laminar. After approximately 25°CA, \( \langle v^2_\varphi \rangle_V \) increases due to turbulence generation by the jet breakup. The evolution of the different cycles is similar, but the values differ significantly.

The spatial location of the turbulent jet breakup process can be deduced from figure 4.10(b), where \( \langle v^2_\varphi \rangle_z \) on horizontal planes are plotted at 36°CA as function of the distance \( z \) from the cylinder head. Cycle 6 breaks up earlier upstream compared to the other cycles as \( \langle v^2_\varphi \rangle_z \) increases faster. In cycles 2 and 4, the breakup takes place farther downstream in the axial direction, as indicated by the slower increase of \( \langle v^2_\varphi \rangle_z \) with \( z \).

It can thus be seen that high \( \langle v^2_\varphi \rangle_V \) (figure 4.10(a)) values at TDC are followed by a jet breakup which happens closer to the cylinder head. The cyclic differences of \( \langle v^2_\varphi \rangle_V \) can result either from the interaction of the incoming jet with the turbulence remaining at TDC or from instabilities in the incoming jet flow. The flow behavior in the valve channel can be characterized by the mean and rms of the velocity magnitude inside the valve annulus as well as the instantaneous profiles extracted along four lines on a plane at \( z = 3.75 \) mm (figure 4.11(a) and (b), respectively). The mean velocity magnitude profiles are very similar for all cycles while the standard deviation displays two peaks of up to 2 m/s close to the channel walls resulting from differences in the boundary layer thickness and the high velocity gradients close to the walls; the relative difference between the cycles is small, and the peaks are approximately at the same location. The instantaneous profiles in figure 4.11(b) are smooth; similar behavior
is observed at all times and for all cycles, which, together with the low Reynolds number \((Re < 1,510)\), confirms that the flow inside the valve channel is always laminar.

In order to investigate the influence of the jet flow angle on the cyclic differences of the jet flow, figure 4.11(c) reports the mean flow angle \(\varphi_{flow} = \arctan(v_z/v_r)\) in the valve channel as function of the piston position. With increasing piston speed after TDC, averaged flow angles of around 28.5° can be observed for all cycles. The deviation from the valve channel angle of 30° is a consequence of the two small recirculation zones formed at the sharp edges at the upper entrance of the valve channel. A relative trend between the cycles cannot be discerned, since the flow angles of all cycles are very similar and the relative order of the cycles is changing. It can thus be concluded that the remaining turbulence in the cylinder at TDC has a stronger effect on the flow in the next cycle compared to the incoming jet.

Figures 4.12(a), (b) and (c) show the azimuthally averaged axial velocity component \(\langle v_z \rangle_\varphi\) at 36°, 90°CA and 144°CA on planes located at the indicated distances from the cylinder head to identify the average radial location of the incoming jet. At 36°CA, the maximum axial velocity and consequently the incoming jet in cycle 4 is located closer to the cylinder axis compared to the lower extremum of the sixth cycle. The axial velocities of cycles 3 and 8 are between the extreme cycles 4 and 6. At the time of maximum piston speed (90°CA), values of \(\langle v_z \rangle_\varphi\) at \(z_{10}\) appear similar all cycles. Starting from \(z_{20}\) clear differences of \(\langle v_z \rangle_\varphi\) can be observed: The jet of cycle 4 is still located closer to the cylinder axis, resulting in lower axial velocities.
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Figure 4.11: (a) Averaged velocity magnitude and standard deviation in the valve channel as a function of the radius for cycles 2 to 8 (C₂ to C₈); (b) Instantaneous velocity magnitudes on a horizontal plane through the valve channel of the third cycle. (c) Averaged flow angle relative the symmetric axis versus the piston position. The data are extracted at z = 3.75 mm and at 90°CA.

close to the cylinder wall. As can be seen in figure 4.9, the incoming jet in the sixth cycle impinges on the wall already at 𝑧₂₀ and flows down along the cylinder wall as indicated by the low axial speeds for 0.8𝑅_c ≤ r ≤ 𝑅_c.

At 144°CA (figure 4.12(c)), the ⟨𝑣₂⟩ᵦ profiles become more similar.

In order to illustrate the effect of cyclic differences in the jet direction at 36°C and 90°CA on the large flow structures at the end of the intake stroke, figure 4.13 compares the flow and pressure fields for cycles 4 and 6 (the cycles exhibiting the most extreme behavior) during the first half of the intake stroke. The dominant flow structure at 144°CA is the vortex ring below the valve, indicated by the pressure iso-surface. While different criteria have been proposed to visualize vortical structures (e.g. λ₂, vorticity magnitude, streamlines in [122]), the pressure iso-surfaces are chosen, as they illustrate more clearly the dominant vortical structures and hence
4.4. Results and discussion

Figure 4.12: Azimuthally-averaged axial velocity component (in m/s) in the cylinder at (a) 36°, (b) 90°CA and (c) 144°CA.

better highlight the vortex ring compared to the other tested methods. The \( \lambda_2 \) and the vorticity magnitude methods reveal a large number of smaller vortical structures (figure 4.9), which, however, are not relevant for the discussion of the dominant structures.

At 144°CA, the piston speed is slower compared to \( V_{p,max} \) (\( V_p = 0.37 \) m/s < \( V_{p,max} \)) and thus the velocity of the incoming jet is also smaller. In the fourth cycle, regions with \( |v| > 2.5 \) m/s, are mainly located around the vortex ring, while in the sixth cycle the velocity field appears to be less organized around the vortex ring and the regions with \( |v| > 2.5 \) m/s extend
all the way to the piston. In this case, the vortex ring below the valve is significantly weaker as indicated by the higher pressure values at the center of the vortex ring. By comparing the dynamics of the vortex rings with the turbulence level at TDC (figure 4.10(a)) and the jet direction (figures 4.12(a) and (b)), the following observation can be made: in cycles with high initial $\langle v^2 \rangle_V$, the jet is located closer to the cylinder wall and the vortex ring appears weaker and more distorted. On the other hand, low initial $\langle v^2 \rangle_V$ values are followed by a relatively more vertically directed jet close to the cylinder axis and a stronger vortex ring.

Figure 4.12 implies that the cycle to cycle variations of azimuthally averaged quantities can change significantly during the intake stroke. In order to quantify cyclic variations, a coefficient of variation (COV) is introduced.
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as follows

\[
COV(\circ CA) = \left\{ \frac{\frac{1}{6} \sum_{n=3}^{8} \sqrt{\left( \langle K_n(\vec{x}, \circ CA) \rangle_{\phi} - \overline{K(\vec{x}, \circ CA)} \right)^2} }{\langle \overline{K(\vec{x}, \circ CA)} \rangle_V} \right\}_V (4.1)
\]

to quantify the difference of individual cycle average \( \langle K_n(\vec{x}, \circ CA) \rangle_{\phi} \) from the azimuthally and ensemble averaged flow field \( \overline{K(\vec{x}, \circ CA)} \) at different times during the intake stroke. \( COV \) values close to zero indicate that the individual cycle means are close to the total mean (e.g. at 144\( ^\circ \)CA, figure 4.12), while high \( COV \) values are related to larger differences of the individual cycle means to the total mean (e.g. at 36\( ^\circ \) and 90\( ^\circ \)CA, figure 4.12).

The \( COV \) during the first half of the intake stroke (figure 4.14(a)) is considerably higher, in agreement with the observations from figure 4.12. The reason for the high cyclic differences at the beginning of the intake stroke is the significant variation in the radial position of the incoming jet. After 90\( ^\circ \)CA, the jet direction is similar for all calculated cycles and the cyclic differences in the mean velocity field decrease rapidly. This observation is in agreement with the experimental observations of [21] reporting significantly lower cyclic differences in the second half of the intake stroke.

The ensemble and volume-averaged turbulent kinetic energy \( \langle \overline{k} \rangle_V (\circ CA) \) during the intake stroke is reported in 4.14(b). In the first half of the stroke, the turbulent kinetic energy level increases as turbulence is produced by the breakup of the incoming jet. From 0\( ^\circ \) to 36\( ^\circ \)CA, the incoming jet is laminar and only a modest increase can be observed. After 36\( ^\circ \)CA, the turbulent
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Figure 4.14: (a) Normalized cyclic variability for discrete piston positions during the intake stroke; (b) cylinder averaged turbulent kinetic energy $\langle \overline{E} \rangle_V$ ($^\circ$CA) (dashed line with symbols) and piston speed (solid line) as a function of piston position.

Kinetic energy increases sharply to reach a maximum value of $1.44\ m^2/s^2$ at $90^\circ$CA and subsequently decreases, but at a slower rate compared to the increase during the first half. The volume averaged turbulent kinetic energy can be seen to scale with twice the piston speed once the flow becomes turbulent ($[3]$).

We now turn to the influence of the vortex ring on the flow field during the exhaust stroke. Figure 4.15(a) shows the vortex ring in terms of pressure iso-surfaces together with the instantaneous velocity field for all cycles at $180^\circ$CA. As indicated in cycle 4, the fluid inside the vortex ring is flowing clockwise around the vortex center and a weaker secondary eddy can be observed at the lower part of the cylinder. In cycles 3 and 4 the vortex ring is horizontal and displays an almost smooth surface, whereas the tilted vortex rings of cycles 5, 6 and 7 are distorted; the relatively smooth pressure
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iso-surfaces of cycles 2 and 8 are also tilted with respect to the symmetry axis.

The dynamics of a stable (cycle 3) and a very distorted vortex ring (cycle 5) is compared in figure 4.15(b) at 207° and 225°CA. As the piston moves upwards, the vortex ring preserves its symmetry and after 225°CA it is pushed out of the cylinder. Compared to the third cycle at 207°CA, the pressure iso-surface of cycle 5 does not have a ring shape and its upper part is pushed out of the cylinder, while the lower part forms the vortex tubes marked as A and B in figure 4.15(b).

The vortex ring structure affects the flow in the cylinder as can be observed in figures 4.16(a) and (b), where the velocity magnitude averaged on planes at different axial positions are plotted at 180°CA and 270°CA of cycles 3 and 5, respectively. At 180°CA of the third cycle, a more pronounced maximum is located at \( z \approx -25\, \text{mm} \), while for cycle 5 a flatter velocity profile results from the distorted vortex ring shown in figure 4.15. At 270°CA (figure 4.16(b)), the velocity profile in cycle 3 becomes almost flat as the vortex ring is pushed out of the cylinder. At the same crank angle degree of cycle 5, a significantly larger average velocity remains inside the cylinder. Therefore, the stability and position of the vortex ring have a dominant effect on the velocity field at TDC and can cause cycle to cycle differences.

A comparison of the velocity distribution in the axial direction for all computed cycles at BDC is shown in figure 4.16(c). Cycles 2 to 4 show higher maximum values (\( \approx 2.5\, \text{m/s} \)) approximately 22-25 \( \text{mm} \) below the
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Figure 4.15: (a) Pressure isosurface and velocity magnitude on a slice (a) at 180°CA for the cycles 2 to 8 and (b) at 207° and 225°CA for the cycles 3 and 5.
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Figure 4.16: Average velocity magnitude versus the axial position in the cylinder: cycles 3 and 5 at (a) BDC (180°) and (b) at the maximum piston speed during the exhaust stroke (270°); (c) cycles 2 to 8 at BDC at 180°.

cylinder head and lower values (≈ 1.0 m/s) close to the piston. In cycles 5 and 6 the peak values decrease and the curves show a broader distribution. After cycle 6 the trend reverses and the maximum values in cycles 7 and 8 are increasing.

4.4.3.3 Multiple cycle behavior

The temporal evolution of the volume-averaged velocity magnitude $\langle |v| \rangle_V$ in the cylinder over the eight computed cycles is plotted in figure 4.17(a); a complete cycle corresponds to 0.3 s. Starting from the value at the end of the previous cycle, $\langle |v| \rangle_V$ increases with the piston speed to reach its maximum shortly after 90° CA and then decreases as the piston decelerates towards BDC. The minimum and maximum values of $\langle |v| \rangle_V$ show significant cycle to cycle differences (table 4.1), which are influenced by the orientation.
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<th>maximum value</th>
<th>deviation from a.m.</th>
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</table>

Table 4.1: Minimum and maximum values of the velocity magnitude for the single cycles. All speeds are in [m/s].

and stability of the vortex ring at BDC (figure 4.15). The minimum value reached at TDC decreases after the second cycle and reaches its lowest value in cycle 4 with a deviation of -20.5% from the arithmetic mean obtained from all cycles. It then increases until cycle 6, reaching a maximum value of 0.378 m/s, and subsequently decreases in cycles 7 and 8. The same trend can be observed for the maximum values. At approximately 270°CA (maximum speed of the upward moving piston marked by circles), the curves develop an inflection point and become flat. Significant differences between the cycles can be observed, which can be attributed to the stability of the vortex ring during the upward piston motion.

Although the limited number of computed cycles does not allow for general conclusions, the following observations can be made. Flow dynamics inside the cylinder are determined by the strength and orientation of the vortex ring generated by the incoming hollow jet. A strong relatively intact horizontal ring aligned with the symmetry axis results in a large coherent
4.4. Results and discussion

Figure 4.17: (a) Time history of the volume averaged velocity magnitude for the eight cycles. (b) zoom in to cycles 4 and 6 with 2-D distributions of the velocity magnitude on central slices at 0°, 90°, 180° and 270°CA.
structure which survives during the expansion cycle and is pushed out of the cylinder by the upward moving piston (figure 4.15, cycles 2, 3, 4, 7 and 8). The fluid remaining in the cylinder at TDC is characterized by a counter-rotating vortex ring close to the corner of the piston and the cylinder wall (figure 4.15, cycle 4). When the ring is significantly distorted (figure 4.15, cycle 5), it affects the flow in the lower half of the cylinder by creating higher radial velocities which survive till the beginning of the next cycle. Two successive cycles are coupled though the conditions at TDC and figure 4.18 shows schematically the sequence of effects in consecutive cycles.

4.4.4 Statistical analysis

After the comparison with the experimental data in the previous section, in this section statistical quantities are reported which are not available from the experimental data. Comparable to section 4.4.2 all quantities reported are obtained by a combination of azimuthal and ensemble (total) averaging of the data from cycles 3 to 8. As discussed in the previous section,
the total average of the radial velocity component \( \overline{v_r} \) affects strongly the development of the jet and the central vortex ring organizing the flow. Mean and rms values on planes at different axial locations and at 36°, 90° and 144°CA are plotted in figure 4.19. At 36°CA the incoming jet is mainly directed in the axial direction, resulting in low radial velocity magnitudes compared to 144°CA. The differences in the sign, with positive \( \overline{v_r} \) values (directed towards the cylinder wall) for \( r/R_c < 0.7 \) and negative \( v_r \) values for \( r/R_c > 0.7 \), can be explained by the influence of the hollow jet. The highest rms velocities are obtained in the two jet shear layers with a small local minimum at \( r/R_c = 0.6 \). Close to the cylinder center the radial rms velocities are in the range between 0.1 and 0.2 m/s. Halfway through the expansion stroke (90°CA) the jet is directed more sidewards, resulting in a high \( \overline{v_r} \) peak value of above 4 m/s at \( z_{10} \) and \( r/R_c = 0.7 \). The negative \( \overline{v_r} \) velocities at \( z_{10} \) and \( r/R_c > 0.85 \) are due to the small recirculation zone at the outer cylinder head (figure 4.4). In the upper part of the cylinder, \( \overline{v_r} \) is positive (below \( z_{30} \)), while farther away from the cylinder head it becomes negative due to the central vortex ring. The rms velocity has values between 0.5 and 1 m/s and is relatively homogeneous in the cylinder except at \( z_{10} \) and \( z_{20} \), where rms velocities of up to 2.1 m/s are reached. At 144°CA the core of the vortex ring is located at approximately \( z_{30} \), characterized by low \( \overline{v_r} \) values at this axial position. Accordingly, at \( z_{10} \) and \( z_{20} \), \( \overline{v_r} \) is positive and below \( z_{30} \) mainly negative. The maximum radial rms velocities are always below 1.2 m/s due to the lower speed of the incoming jet.

The spatial distribution of the mean turbulent kinetic energy during
the intake stroke is plotted in figure 4.20. At 45°CA the maximum value of 2.57 m²/s² is at the jet tip. With increasing piston speed, $k_{max}$ increases to 6.25 m²/s² at 67.5°CA. At 90°CA, $k$ is produced at the outer shear layer of the incoming jet reaching a maximum of 7.15 m²/s². During the second half of the intake stroke, the incoming jet impinges directly on the cylinder wall, increasing the dissipation rate in this region and decreasing $k_{max}$. During the exhaust stroke, $k$ is more homogeneously distributed inside the cylinder and decreases continuously until the TDC of the next cycle.

Components of the Reynolds stresses at 36°, 90° and 144°CA are shown in figure 4.21. The $r_r v'_r$ and $z_\phi v'_\phi$ components are found to be almost zero.
at all times in the whole domain (as a consequence of the axis-symmetry of the geometry and of averaging) and are not shown. At 36°CA (figure 4.21(a)), the maximum stress in the $z$-direction is located at the inner shear layer of the incoming jet where the axial velocity component is larger. The maximum value of the axial stress ($3.21 \text{ m}^2/\text{s}^2$) is significantly larger than the other components. Due to the higher radial velocities and variations in the jet direction in individual cycles, the largest stresses in the $r$-direction are located in the upper shear layer. In contrast to $\overline{v'_z v'_z}$ and $\overline{v'_r v'_r}$, $\overline{v'_r v'_\phi}$ (which is used as an indicator for turbulence generation, since it is mainly formed due to the turbulent redistribution of $v_z$ and $v_r$ to $v_\phi$) is almost zero in the shear layers of the incoming jet and its maximum value ($0.61 \text{ m}^2/\text{s}^2$) is reached around the jet tip. The non-zero values of $\overline{v'_r v'_z}$ indicate an anisotropic flow behavior in the jet shear layers. The high cyclic fluctuations at 90°CA (figure 4.21(b)) can be seen in the stress tensor components: the axial component maximum shifts close to the cylinder wall, reflecting the
4. DNS of Multiple Cylces in an Engine-like Geometry

large cyclic differences in the jet position reported in figure 4.12, while the radial component maximum remains at the upper shear layer of the jet. The maximum of the $v'_r v'_r$ component is located in the upper shear layer close to the cylinder wall. The higher values of the shear stress component $v'_r v'_\phi$ indicate increased anisotropy level with higher piston speed.

Later in the cycle, nonzero stresses are found in larger parts of the domain (figure 4.21(c) at 144°CA) and the variation in the maximum values of the main components becomes smaller, as expected from the lower cycle to cycle variation (figure 4.14). In the central part of the cylinder, lower values of the stress component $v'_z v'_z$ compared to $v'_r v'_r$ and $v'_\phi v'_\phi$ can be observed. It should be noted, however, that due to the smaller sample size the statistical values close to the symmetry axis ($r/R_c < 0.3$) are not fully converged.

A quantitative comparison of the turbulent kinetic energy and the stress tensor data is provided in figure 4.22. During the intake stroke the flow anisotropy is more pronounced at $z_{10}$ and $z_{20}$ but is reduced closer to the piston. The peak of the $v'_z v'_z$ component close to the wall at 90° and locations $z_{20} - z_{40}$ can be attributed to cyclic differences in the jet direction as reported in the previous section. The stress component $v'_r v'_r$ shows faster decaying values towards the cylinder wall compared to $v'_z v'_z$ and $v'_\phi v'_\phi$, which can be explained by the dampening effect for wall normal stress components [120].

Overall the stress tensor shows a complex anisotropic fluctuation field. Similar to the findings of [123], the turbulence field in the cylinder at the
4.4. Results and discussion

Figure 4.21: Reynolds stresses $[m^2/s^2]$ at (a) 36°, (b) 90° and (c) 144°CA.
Figure 4.22: Turbulent kinetic energy and Reynolds stresses (in \([m^2/s^2]\)) at 36°, 90° and 144°CA.
4.4. Results and discussion

time of maximum piston speed shows a very anisotropic behavior, since
turbulence is mainly produced by the jet breakup. With decreasing piston
speed less turbulence is produced and the turbulent flow becomes more
homogeneous and isotropic close to BDC.

Figure 4.23 shows the integral length scales of $v_\varphi$ at 36°, 90° and
144°CA of the third cycle, which displayed small mean field variations in the
azimuthal direction. The values close to the cylinder center ($r/R_c < 0.3$) are
not shown, because of the insufficient number of statistically independent
sample points in this region. The integral length scale is calculated based
on the velocity component in azimuthal direction, since its mean value is
always close to zero and thus the results are less dependent on the cyclic
variability of the flow field. The integral length scale at a single point is
computed by extracting $v_\varphi$ along a circle at a fixed radial and axial position,
and calculating its autocorrelation. According to [124], the integral length
scale can be defined as the distance where the autocorrelation decreases to
10% of its maximum value. In the outer region of the cylinder and the pis-
ton wall the integral length scales at 36°CA are larger than 5 mm, whereas
around the incoming jet, they decrease to 1.2 mm. At 90°CA, the integral
length scales in the whole cylinder drop below 4 mm, with the exception of
the center of the vortex ring and the area close to the outer cylinder head.
The smallest values of approximately 0.9 mm are located in the incoming
jet and at the cylinder wall. Due to the lower piston speed at 144°CA the
spread in the integral length scales is reduced and ranges between 2 and
4 mm, except for the incoming jet which has scales of approximately 1.5
Figure 4.23: Integral length scales of the azimuthal velocity component in the third cycle at 36°, 90° and 144°CA.

...mm. The smallest scales are always located in the area of the jet breakup and a correlation with the piston speed can be observed. Towards BDC the differences in the integral length scale in the cylinder become smaller. The grid resolution in LES must be smaller than the integral length scale \[120\], the values provided in figure 4.23 indicate the resolution requirements for LES simulations of this setup.

### 4.4.5 Cause-and-effect relationships of CCVs

In this section three additional cycles are calculated in order to increase the number of statistical relevant cycles for the investigation of the cause-and-effect relationships of CCVs. In the previous section 4.4.3 the flow field at TDC, the trajectory of the incoming jet and the orientation and stability of the vortex ring have been identified to be the main physical mechanism for
the cyclic variability. In section 4.4.5.1 the influence of the flow field at TDC on the jet direction is investigated in detail, followed by the description of the correlation between the jet flow and the vortex ring formation in section 4.4.5.2. Finally the influence of the vortex ring on the flow field at TDC of the next cycle is assessed in section 4.4.5.3.

4.4.5.1 Influence of the initial conditions on the jet trajectory

The cyclic variations in this setup result from the interaction of the hollow jet flow with the formation and relaxation of the large central vortex ring. In this section the influence of the remaining vortex ring from the previous cycle on the hollow jet of the actual cycle is discussed.

In figure 4.24 the radial velocity at TDC ($0^\circ$CA) and the pressure distribution at $22.5^\circ$CA are plotted on x-z slices for cycles 3 and 7. For $v_r > 0$ (red color) the fluid flows towards the cylinder wall and for $v_r < 0$ (blue color) the fluid moves towards the cylinder center. The radial velocity is not defined at the cylinder axis, which appears as discontinuity. The radial velocities in cycle 3 (left image) are relatively small compared to cycle 7 (right image), where $v_r$ is negative on the left and positive on the right side, resulting in the flow direction indicated by the arrows.

At $22.5^\circ$CA the downwards moving piston creates an accelerating jet flow into the cylinder. The low pressure regions on both sides of the jet tips of cycle 3 and 7 (figure 4.24(b)) correspond to the vortex ring centers shown in figure 4.4. In cycle 3, the inner low pressure regions on both sides are larger and have a lower minimum pressure value compared to the outer
regions. This is due to different nozzle exit angles for the inner and the outer side, since according to Shariff and Leonard [71] the strength of the vortex ring is influenced by the angle of the nozzle exit.

The low pressure regions in cycle 7 differ at both sides. At location B1, similar to cycle 3, the inner low pressure region is more pronounced, while at B2 the two regions are approximately equal in size and have a similar minimum pressure. This is due to the directed radial velocity at TDC, which inhibits the roll-up of the nozzle boundary layer at the leading edge. This is in agreement with the findings in Sau and Mahesh [73], which showed that the vortex ring side facing the cross flow is weaker compared to the opposite side.

In figure 4.25 the velocity magnitude of cycles 3 and 7 is displayed on $x\,\,z$ slices at 22.5°, 45° and 67.5°CA. For cycle 3, the direction of the incoming jet at 22.5° is defined by the valve channel angle. At 45° and 67.5°CA the low pressure region inside the hollow jet cone forces the jet towards the cylinder center preventing a jet impingement on the cylinder wall. At 67.5°CA the jet impinges on the piston, recirculates in the cylinder center and forms a doughnut-shaped central vortex ring.

In contrast to cycle 3, significant differences in the jet trajectory between the two shown sides can be observed for cycle 7. While the jet trajectory at the left side is comparable to the one of cycle 3, the jet on the right side flows straight towards the cylinder wall (position B3). This can be attributed to the comparable pressure levels in the inner and outer recirculation zones. As a consequence, the jet trajectory is strongly influ-
Figure 4.24: (a) Instantaneous radial velocity on a axial slice at TDC for cycles 3 and 7; (b) pressure distribution on a axial slice at 22.5°CA for cycle 3 and 7.

enced by the cross flow resulting from the radial velocity at TDC. A strong influence of cross-flows on trajectories of circular jets is also reported in Mahesh [70].

The relation between \( v_r \) at TDC and the jet trajectory is so far only illustrated for two cycles. In the following it will be shown that this correlation can be observed for all calculated cycles and in all azimuthal directions. For this comparison it is necessary to reduce the amount of data and extract characteristic values for the radial velocity at TDC and the corresponding
4. DNS of multiple cycles in an engine-like geometry

Figure 4.25: Instantaneously velocity magnitude on a central slice at \(22.5^\circ\) and \(45^\circ\)CA of cycles 3 and 7.
jet radius. The characteristic values are derived as a function of the azimuthal angle, \( \varphi \), since, as seen before, the radial velocity at TDC and the jet radius vary in the azimuthal direction.

The radial velocity at TDC is averaged according to:

\[
v_{r,TDC}(\varphi) = \frac{1}{37.5} \int_{0}^{37.5} r \left[ \frac{1}{11.25} \int_{-11.25}^{0} v_r(\varphi, r, z) \, dz \right] \, dr \quad (4.2)
\]

The averaging in axial direction is applied between 0 and -11.25 mm (see the dashed line in figure 4.24 (a)). The threshold of -11.25 mm is chosen, since mainly the flow field in the entry section of the cylinder is interacting with the incoming jet. The sensitivity to this threshold is low, as shown in figure 4.26(a) where different threshold values are used.

![Figure 4.26: (a) Effect of threshold on the radial velocities profiles at TDC; (b) jet position tracked by an iso-surface of \( v_z = -2.5 \, m/s \) for \( \varphi = \pi \) in cycle 7 at 45°CA.](image)

The jet radius is calculated at 45°CA, since before the jet speed is too low and after 60°CA the jet radius is influenced by the cylinder wall. The iso-surface \( v_z = -2.5 \, m/s \) is chosen to define the jet boundary \( r_j(\varphi, r, z) \) (figure...
The averaged jet position $r_j(\varphi)$ is then computed by averaging the iso-surface radii in axial and radial direction:

$$r_j(\varphi) = \frac{1}{37.5} \int_{0}^{37.5} r \left[ \frac{1}{37.5} \int_{-37.5}^{0} r_j(\varphi, r, z) \, dz \right] \, dr$$  \hspace{1cm} (4.3)

The threshold $v_z$ value is chosen so that the iso-surface is located in the shear layers of the incoming jet. The calculated jet radius is insensitive to the threshold value, since the velocity gradients in the jet shear layers are very large. For a threshold range between -3 m/s and -2 m/s the calculated average jet radius varies less than 1%. The threshold in axial direction (37.5 mm) is chosen large enough to contain the full iso-surface contour in the cylinder.

A comparison of the radial velocity at TDC ($v_{r,TDC}(\varphi)$) and the jet radius at 45°CA ($r_j(\varphi)$) for all cycles is shown in figure 4.27(a). In all graphs a clear correlation between the radial velocity at TDC (dashed blue line) and the jet radius at 45°CA (solid red line) can be seen. For all cycles and azimuthal directions larger radial velocities at TDC are followed by also larger jet radii at 45°CA. This can be very clearly seen for cycle 6, where for $0 < \varphi < \pi$ $v_{r,TDC}(\varphi)$ and $r_j(\varphi)$ are relatively low while between $\pi < \varphi < 2\pi$ $v_{r,TDC}(\varphi)$ and $r_j(\varphi)$ are both increased. This behavior is plausible, since (as shown in the figures 4.24 and 4.25) a positive $v_{r,TDC}(\varphi)$ pushes the jet trajectory $r_j(\varphi)$ towards the cylinder wall. In order to connect the visual observations with the extracted curves in figure 4.27(a) the positions A3
and B3 correspond to the locations A3 and B3 in figures 4.24 and 4.25. At point A3 in figure 4.27 \( v_{r,TDC}(\varphi) \) is close to zero and the jet radius \( (r_j(\varphi)) \) normalized by the cylinder radius \( r_c \) is equal to 0.62. In contrast to this at point B3 in cycle 7 \( v_{r,TDC}(\varphi) \) is +0.225 [\text{m/s}] and the jet radius is 0.665.

Figure 4.27(b), which illustrates the axial vortex ring position as a function of the azimuthal direction and will be discussed later in this work (section 4.4.5.2). It is plotted next to figure 4.27(a) in order to later show the correlations between the two graphs.

The correlation of the cyclic averaged radial velocity at TDC with the jet radius at 45\(^\circ\)CA is shown in figure 4.28. The cyclic means derived by averaging \( v_{r,TDC}(\varphi) \) and \( r_j(\varphi) \) between 0 and 2\(\pi\) are in the following denoted by \( < v_{r,TDC} >_{\varphi} \) and \( < r_j >_{\varphi} \). The averaged quantities in figure 4.28 show a nearly linear correlation between the cycles, with a correlation coefficient of \( R^2 = 0.95 \). It can clearly be seen that positive averaged radial velocities (directed towards the cylinder wall) are followed by larger jet radii, while accordingly smaller \( < v_{r,TDC} >_{\varphi} \) are followed by smaller \( < r_j >_{\varphi} \) values. The high \( R^2 \) value is in the first moment surprising, since the after 45\(^\circ\)CA the jet velocities are significant larger compared to the magnitudes of the radial velocity at TDC (see figure 4.25 and 4.24). The strong correlation results from the influence of the radial velocity to the jet trajectory during the very early intake stroke (between TDC and 20\(^\circ\)CA), when the jet velocity is comparable to the radial velocity at TDC.
Figure 4.27: (a) $v_{r,TDC}$ (0°CA) and $r_j$ (45°CA) versus the azimuthal angle; (b) $z_v$ versus the azimuthal angle at 180°CA. The axial vortex ring position will be explained later in section 4.4.5.2.
4.4. Results and discussion

4.4.5.2 Influence of the jet flow on the vortex ring formation

In the previous section the influence of the flow field from cycle $n-1$ on the jet trajectory in cycle $n$ was observed. Based on this in this section the influence of the hollow jet on the vortex ring formation process within cycle $n$ is discussed.

The jet center is a good indicator of the asymmetry of the flow field which, as will be shown later, is essential for the stability of the large central vortex ring. The jet centers of all cycles are computed based on the jet radii $r_j(\varphi)$ defined in equation 4.3. The positions are derived by first transforming the radial jet positions $r_j(\varphi)$ into Cartesian coordinates and then average the resulting $x$ and $y$ coordinates. The jet flow of cycle 7 is indicated in figure 4.29(a), showing the velocity magnitude on a horizontal slice at $45^\circ$CA. It can be seen, that the jet center is shifted to the upper left side.

Figure 4.28: $<v_{r,TDC}>\varphi$ at TDC ($0^\circ$CA) versus the jet radius ($<r_j>\varphi$) at $45^\circ$CA.
with respect to the symmetry axis. The jet center positions of all cycles are illustrated by the squares in figure 4.29(c); the numerical values are given in table 4.2.

<table>
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Table 4.2: Radius and angle of the jet center positions at 45°C CA.

The shift in the jet center is connected to the radial velocity at TDC, which is exemplarily shown in figure 4.29(b) for cycle 7. The majority of the velocity vectors are directed towards the upper left side, which 45°C CA later causes the shift in the jet center. The average direction and magnitude of the radial velocity at TDC can be quantified by using the averaged radial velocity defined in equation 4.2. \( v_{r,TDC}(\varphi) \) can be interpreted as a series of vectors with the magnitude \(|v_{r,TDC}(\varphi)|\) for the angle \(\varphi\). The sum of all radial velocity vectors \(v_{r,TDC}(\varphi)\) result in an averaged radial velocity vector, which in the following will be denoted as \(\vec{v}_{r,TDC}\).

The values of \(\vec{v}_{r,TDC}\) are given in table 4.3 and the vectors of all cycles are plotted in figure 4.29(c). A good correlation between \(\vec{v}_{r,TDC}\) and the jet centers (squares in figure 4.29(c)) can be observed for all cycles except cycle 6 where the azimuthal direction agrees well but the length of \(\vec{v}_{r,TDC}\) is relatively large compared to the later jet off-center radius. The reason for
4.4. Results and discussion

<table>
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<th>4</th>
<th>5</th>
<th>6</th>
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<tbody>
<tr>
<td>$</td>
<td>\vec{v}_{r,TDC}</td>
<td>$</td>
<td>0.008</td>
<td>0.024</td>
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<td>11</td>
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<td>$</td>
<td>\vec{v}_{r,TDC}</td>
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Table 4.3: Magnitude [m/s] and angle [rad] of the initial radial velocity vector at 0°CA.

this discrepancy is the limiting effect of the cylinder wall for very high jet radii.

The effect of the shifted jet center on the flow field is shown in figure 4.30 where the flow field at 45°CA in cycle 5 is shown by velocity vectors. Comparable to the jet center the approximate position of the stagnation point (indicated by the red crosses in figure 4.30) is shifted in negative x and positive y-direction. This results in asymmetry in the vortex ring formation process causes a rotation of the vortex ring axis, which as will be shown below.

The central vortex rings for cycles 2 to 11 are illustrated in figure 4.31 by pressure iso-surfaces. The value of the pressure iso-surfaces ($p_{iso}$) is adjusted for each cycle in order to better visualize the shape of the vortex ring. Large differences in the surface shape and the spatial orientation of the vortex rings can be observed. The vortex rings of cycle 3, 4 and 10 are horizontal and relatively smooth, while the rings of cycle 6 and 11 are strongly distorted.

When comparing the jet centers with the spatial vortex ring orienta-
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Figure 4.29: (a) Instantaneous velocity magnitude of cycle 7 on a horizontal slice at z = -10 mm and 45°CA; (b) velocity vectors at z = -4 mm at TDC of cycle 7; (c) squares: x and y coordinates of the jet center positions at 45°CA; vectors: averaged $v_{r,TDC}$ velocity vectors at TDC. (vector length of cycle 6 multiplied by 0.5).

In order to quantify the correlation between the hollow jet flow and
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Figure 4.30: Flow field on slices through the x and y axis at 45°CA in cycle 5.

the vortex ring for all cycles the axial vortex ring position \((z_v(\phi, r, z))\) is defined at axial locations where \(p < -1.3 \text{ Pa}\). The averaged axial vortex ring position \(z_v(\phi)\) is then calculated by averaging in axial and radial direction.

\[
\frac{1}{37.5} \int_0^{37.5} r \left[ \frac{1}{90} \int_{-90}^{0} z_v(\phi, r, z) \, dz \right] \, dr \quad (4.4)
\]

The pressure threshold value has been chosen low enough to select only locations close to the vortex ring center and high enough to identify locations in all cycles and azimuthal directions.

The axial vortex ring position for all cycles is plotted in figure 4.27(b). When comparing the curves of figure 4.27 (a) and (b) it can be seen that higher radial velocities \(v_{r,TDC}(\phi)\) at TDC are followed by larger jet radii \(r_j(\phi)\) at 45°CA, which result in a higher vortex ring position \(z_v(\phi)\) at BDC. Thus the aforementioned correlation between jet center and vortex ring orientation applies for all cycles in all azimuthal directions. The correlation

...
between $r_j(\varphi)$ at 45°CA and $z_v(\varphi)$ at BDC is quantified in table 4.4. A low correlation coefficient ($R^2$) indicates a relatively symmetric flow field (cycles 2, 3, 4, 9 and 10), while higher $R^2$ values (above 0.5) can be observed in cycles with relatively asymmetric flows (cycles 5, 6, 7 and 11).
4.4. Results and discussion

<table>
<thead>
<tr>
<th>Cycle</th>
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<th>5</th>
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<tr>
<td>$R^2(r_j(\varphi), z_v(\varphi))$</td>
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<td>0.001</td>
<td>0.007</td>
<td>0.658</td>
<td>0.548</td>
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Table 4.4: Correlation coefficients ($R^2$) between $r_j(\varphi)$ at 45°CA and $z_v(\varphi)$ at BDC for all calculated cycles.

4.4.5.3 Influence of the vortex ring on the radial velocity at TDC of the next cycle

Following the discussion of the correlation between hollow jet and vortex ring in each individual cycle $n$, in this section the influence of the vortex ring dynamics on the flow field at TDC of cycle $n+1$ is investigated. This is the final step in the discussion of a full cycle, since the influence of the flow field at TDC on the dynamics of the hollow jet was discussed in section 4.4.5.1.

In order to compare individual cycles, the vortex ring angle (indicated as $\beta$ in the fifth cycle in figure 4.31) and the vortex ring strength (quantified by $p_{\text{min}}$) are obtained as follows: The vortex ring angle $\beta$ is the angle between the horizontal (x-y) plane and the line defined by the highest and the lowest vortex ring position: $\beta = \arctan \left( \frac{z_v(\varphi_{\text{high}})-z_v(\varphi_{\text{low}})}{r_v(\varphi_{\text{high}})+r_v(\varphi_{\text{low}})} \right)$, where $\varphi_{\text{high}}$ and $\varphi_{\text{low}}$ are the azimuthal angles of the highest and lowest axial position, as shown in figure 4.27(b) and $r_v(\varphi)$ is the averaged radial vortex ring position for the azimuthal direction $\varphi$. According to Jeong and Hussain [122] the vortex ring strength can be quantified by the pressure minimum in the vortex ring core. The azimuthally averaged minimum pressure ($p_{\text{min}}$) is
4. DNS of multiple cycles in an engine-like geometry

<table>
<thead>
<tr>
<th>Cycle</th>
<th>2</th>
<th>3</th>
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<td>11</td>
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<tr>
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<td>18.8</td>
<td>16.3</td>
<td>11.6</td>
</tr>
<tr>
<td>( p_{\min} )</td>
<td>-6.115</td>
<td>-8.455</td>
<td>-5.69</td>
<td>-6.59</td>
<td>-5.14</td>
</tr>
</tbody>
</table>

Table 4.5: Vortex ring angle (\( \beta [^\circ] \)) and averaged minimum pressure (\( p_{\min} \) [\( Pa \)]) at BDC.

defined as: \( p_{\min} = \frac{1}{2\pi} \int_{2\pi}^{0} \min(p(\varphi)) \) d\( \varphi \), where \( \min(p(\varphi)) \) is the minimum pressure as function of the azimuthal direction \( \varphi \). The resulting values for \( \beta \) and \( p_{\min} \) are shown in table 4.5.

The effect of the vortex ring dynamics on the radial velocity in the next cycle is illustrated in figure 4.32 showing the vortex rings of cycle 3 (smallest \( \beta \)) and 5 (largest \( \beta \)) at 180°, 207° and 225°CA. The velocity magnitude |\( v \)| is plotted on x – z planes. During the exhaust stroke of cycle 3, the vortex ring remains axis-symmetric and is almost pushed out of the cylinder at 225°CA. The strongly tilted vortex ring of cycle 5 (\( \beta = 30.65^\circ \)) on the other hand, shows an interesting dynamical behavior during the exhaust phase. From 180° to 207°CA the upper half of the vortex ring is pushed out of the cylinder while the remaining lower part creates two new vortex tubes (positions A and B in figure 4.32). These two vortex tubes are not connected and extend all the way from cylinder wall to the valve gap.

The effect of the vortex tubes on the flow field in cycle 5 is illustrated in figure 4.33(a), which shows velocity vectors on a horizontal slice 15 mm below the cylinder head at 250°CA. The fluid rotates around the pressure
4.4. Results and discussion

Figure 4.32: Pressure isosurface and velocity magnitude on a slice during the exhaust stroke at 180°CA, 207°CA and 225°CA for cycles 3 (smallest $\beta$) and 5 (largest $\beta$).
iso-surfaces inducing a flow in negative y-direction at the cylinder center. This flow is also visible at TDC of cycle 6, which is indicated by higher radial velocities in the negative y-direction ($3.5 < \varphi < 6$) in figure 4.27(a) and an angle of the radial velocity vector ($\overrightarrow{v_{r,TDC}}$) of $\varphi = 4.911$ (table 4.3).

In figure 4.33(b) it is shown that the aforementioned correlation between the vortex ring angle $\beta$ of one cycle $n$ and the radial velocity vector at TDC of the following cycle $n+1$ holds for all calculated cycles. Less tilted vortex rings at BDC are followed by smaller $|\overrightarrow{v_{r,TDC}}|$ values at TDC of the following cycle. Deviations from the correlation are due to uncertainties in the definition of the plane on the strongly tilted vortex rings and differences in the vortex ring strengths, which also influence the imposed radial velocity.

The effect of a stable vortex ring (as in cycle 3) on the radial velocity at TDC of cycle 4 is shown in figure 4.34(a). The large central vortex ring in the upper half of the cylinder creates a secondary counter clockwise vortex ring close to the piston (indicated by the arrow). The strength of the secondary vortex ring correlates with the strength of the central vortex ring ($p_{min}$). At TDC of cycle 4 the central vortex ring is fully pushed out and the secondary vortex ring imposes a negative radial velocity at the cylinder head. This is the reason for the negative $< v_{r,TDC} >_{\varphi}$ value of cycle 4 in figure 4.28. In addition the axis-symmetric vortex ring in cycle 3 during exhaust is followed by a relatively symmetric jet trajectory in cycle 4 (figure 4.29(c)).

In figure 4.34(b) the vortex ring strength ($p_{min}$) and the azimuthal
Figure 4.33: (a) Vortex ring during the outlet phase of cycle 5 at 250°CA. The vectors show radial and azimuthal velocity vectors on a plane 15 mm below the cylinder head; (b) $p_{\text{min}}$ of cycle $n$ versus $<v_{r,TDC}>_{\varphi}$ of cycle $n+1$.

Averaged radial velocity ($<v_{r,TDC}>_{\varphi}$) at TDC of the next cycle are correlated for the cycles 2 to 10. A tendency for the calculated cycles can be seen: stronger vortex rings (lower $p_{\text{min}}$) are followed by lower averaged radial velocities. The reason for this behavior is, that according to figure 4.34(a) a stronger central vortex ring imposes a stronger secondary vortex ring. This secondary ring remains in the cylinder during the exhaust stroke and creates a negative radial velocity close to the cylinder head at TDC of the next cycle.
4. DNS of multiple cycles in an engine-like geometry

Figure 4.34: (a) Azimuthal averaged velocity magnitude at 180° (BDC) of cycle 3 and 0° CA (TDC) of cycle 4; (b) $\beta$ of cycle $n$ versus the $|\bar{v}_{r,TDC}|$ of cycle $n+1$

4.5 Summary and conclusions

Multiple cycles of the incompressible flow in the valve/piston assembly studied experimentally by Morse, Whitelaw, and Yianneskis [1] are investigated using direct numerical simulation. The adequacy of the grid resolution is first assessed by comparing four resolutions for which converging results are found for vorticity length scales, mean and fluctuation velocities. In addition, very good agreement is found with all available measurements in terms of flow structures as well as mean and rms velocities at different piston positions and measurement locations.

During the first half of the intake stroke the flow field is dominated by the incoming hollow jet flowing through the valve with a velocity changing
in magnitude according to the piston speed. The flow in the valve channel remains laminar during the whole cycle and is shown to have only a minor effect on cyclic variations for this setup. In contrast to this the trajectory of the incoming jet is significantly influenced by the remaining radial velocity from the previous cycle. A nearly linear relationship between the radial velocity at TDC and the jet direction at 45°CA can be shown. In all calculated cycles the jet creates during intake one large central and two smaller vortex rings at the corners of the cylinder liner with the cylinder head and the piston. The stability and orientation of the large central vortex ring shows a strong dependence on the symmetry of the hollow jet flow. If the central jet position overlaps with the geometrical center a stable and axisymmetric vortex ring is formed. If the offset between symmetry axis and central jet position becomes too large the vortex ring gets tilted due to an asymmetry in the vortex ring formation process. Tilted vortex rings are only partially pushed out by the upward moving piston leaving larger coherent structures, which impose a non-symmetric flow in radial direction at TDC of the next cycle. In contrast to this, almost axis-symmetric horizontal vortex rings remain unchanged and are eventually pushed out through the open valve, leaving an axisymmetric counter-clockwise rotating vortex at the liner/piston corner at the TDC of the next cycle. In turn, the radial velocity at TDC affects the jet trajectory and flow dynamics of the subsequent cycle, resulting in strong cycle to cycle variations in the investigated engine-like geometry.

The observed dynamic coupling can be directly applied to engine types
with a similar intake valve configuration (like e.g. two-stroke engines), but
differences are expected compared to tumbling or swirling intake configura-
tions. Nevertheless, the results form the basis for future investigations of
CCVs in real engine geometries and some of the found correlations (e.g. the
interaction between in-cylinder flow field and jet trajectory) appear promis-
ing to apply also in real engine geometries. In addition, the results can be
used for the direct assessment of whether different LES models and mesh
resolutions are capable of capturing the CCVs in the setup considered here.
Time and location of possible deviations can be precisely identified, which
can be used to validate and improve LES turbulence models for ICEs.

The mean and rms radial velocities, turbulent kinetic energies, Reynolds
stress components, and integral length scales were also extracted from the
DNS data. In the first half of the intake stroke turbulence is mainly pro-
duced at the shear layers and by the jet breakup, and is highly anisotropic.
With the decelerating piston in the second half of the intake stroke, the role
of the jet weakens and turbulent fluctuations are distributed more homo-
geneously inside the cylinder. The azimuthal direction is especially suited
for comparisons with LES calculations, since it is independent from the
averaging process. Based on the integral length scale, the minimum mesh
resolution requirements for LES calculations can be estimated, which peak
in the shear layers of the incoming jet at 90°CA and at the walls.
Chapter 5

DNS of the compression stroke under engine-like conditions

5.1 Introduction

In this section we turn to the direct numerical simulation of the compression stroke under engine relevant conditions. The initial conditions are derived from a precursor DNS of the intake stroke which accounts for thermal and composition mixing. This procedure avoids the use of artificial initial conditions for flow, temperature and composition based on predefined spectra commonly employed in the literature (see, for example [56]).

The section is structured as follows: in the first part the numerical setup and the derivation of the initial conditions are described. Subsequently, the evolution of the flow, temperature and composition fields during the compression stroke are investigated. Of special interest are the fields around TDC, where the mixture is expected to autoignite (section 5.4.2). The focus in this chapter lies on the investigation of flow and tempera-
ture close to the walls. Thus, in section 5.4.3 the velocity and the thermal boundary layer are analyzed and a detailed discussion of wall heat transfer is presented in section 5.4.4. Finally, the influence of thermally stratified conditions at BDC are isolated and assessed in section 5.4.5. Segments of this chapter appeared in Schmitt et al. [125].

5.2 Numerical setup

For the simulation of the compression stroke the valve is closed at BDC, which corresponds to the time instant of zero mass flux through the valve. The computational domain reduces to the cylindrical part of the geometry from the previous chapter shown schematically in figure 5.1(a). The compression ratio is set to CR = 12 so that the piston moves from 90 mm (BDC) to 7.5 mm (TDC). The turning speed is adjusted to 560 rpm in order to maintain the same Reynolds number as in the multiple cycle flow simulation in chapter 4. For the flow field zero velocity Dirichlet boundary conditions are imposed at all walls with the exception of the piston surface which moves with the piston velocity. A constant temperature of 500 K is set on all boundaries and zero flux boundary conditions are specified for the species.

Two grids are constructed by extruding horizontal slices in the axial direction. The first grid (mesh 1) containing 2436 spectral elements on the $x - y$ plane (figure 5.1(b)) and 54 layers of elements in the axial direction clustered towards the piston and cylinder head is used for crank angles between 180 and 306°. For a polynomial order of $N = 9$, an average axial
5.2. Numerical setup

resolution of 180 \( \mu m \) at BDC and 50 \( \mu m \) at 306° is obtained with a total of approximately 90 million nodes. In the radial and azimuthal direction the resolution is approximately 150 \( \mu m \), while refinements close to the walls results in a resolution of better than 13.8 \( \mu m \). In order to satisfy the increased resolution requirements during the last phase of the compression stroke (> 306°CA), a second grid (mesh 2) with 3410 elements on the horizontal slice and 30 layers of elements in the axial direction is used and the fields are interpolated using high order spectral interpolation. By increasing the polynomial order to \( N = 11 \) (corresponding to 135 million nodes) the average axial resolution is 110 \( \mu m \) at 306° and 30 \( \mu m \) at TDC. In the radial and azimuthal directions the resolution is 95 \( \mu m \) in the bulk of the domain and better than 9.75 \( \mu m \) close to the walls.

The resolution requirements until 310°CA are comparable to those of the incompressible flow simulation (chapter 4), where they were assessed
by a mesh resolution study and comparison with experimental data. As described below, with increasing pressure the size of the smallest scales decrease, resulting in significantly increased resolution requirements close to TDC. The Kolmogorov length scale \( \eta_K = (\nu^3/\varepsilon)^{1/4} \) at TDC is \( \eta_K = 12.8 \mu m \), where \( \varepsilon = 2\nu \langle s_{ij}s_{ij} \rangle \) is the dissipation rate computed from the strain tensor \( s_{ij} = \partial u_i/\partial x_j + \partial u_j/\partial x_i \). At TDC the radial and azimuthal resolution is approximately \( 7.5\eta_K \), while in the axial direction \( dz \approx 2.3\eta_K \). For the employed high order spectral element discretization method this is enough to capture accurately most of the dissipation, and thus provide reliable first and second order statistics (Moin and Mahesh [14]). The resolution is also fine enough to resolve the mixing scales (i.e. the Batchelor scale \( \eta_B = (\nu D^2/\varepsilon)^{1/4} \) and the Obukhov-Corrsin scale \( \eta_{OC} = (D^3/\varepsilon)^{1/4} \)), which are larger than \( \eta_K \) since the Schmidt number is \( Sc = \nu/D < 1 \).

The mesh resolution in wall-normal units is reported in table 5.1. The average grid resolutions of the three spatial directions (\( \Delta r, \Delta r\varphi \) and \( \Delta z \)) are non-dimensionalized as follows: \( \Delta r^+ = \frac{\Delta r}{\nu_{cyl}} \sqrt{\tau_w/\rho_{cyl}} \), where \( \rho_{cyl} \) and \( \nu_{cyl} \) are the average density and the viscosity in the cylinder, \( \tau_w \) is the average magnitude of the wall shear stress and \( \Delta r \) is the average resolution in the radial direction. The distance between the first grid point and the wall is denoted by \( \Delta w_n \). For the non-dimensionalization of \( \Delta w_n^+ \) the density and viscosity are derived based on the fixed wall temperature of 500 K. The resolution employed in this work is comparable to the DNS study of Nicoud [82], indicating a sufficient resolution in order to resolve the wall boundary layer. An overview about resolutions in papers studying wall
5.2. Numerical setup

<table>
<thead>
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<th>P O</th>
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<th>Δrφ⁺</th>
<th>Δz⁺</th>
<th>Δw_n⁺</th>
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<td>&lt; 6</td>
<td>&lt; 6</td>
<td>&lt; 3</td>
</tr>
</tbody>
</table>

Table 5.1: Spatial mesh resolution in wall-normal units. (P O = Polynomial Order)

boundary layers is given in the introduction of Araya and Castillo [126],
which studies velocity and thermal boundary layers in channel flows.

The conservation equations are integrated in time using the third-order
mixed implicit-explicit scheme. In space the chosen polynomial order results
in a discretization order of 9 until 306°CA and 11 until 360°CA [109]. The
time step is adjusted during the simulation in order to respect a fixed maxi-
mum Courant number of 0.5. The simulations were performed on the Cray
XE6 system of the Swiss Supercomputing Center (CSCS) and required ap-
proximately 353,000 CPUh for the simulation of one compression cycle.

Notations:

For temperature, statistics are also collected within an inner cylinder
of radius 30 mm and axial extend (from the cylinder to the piston) of 7.5
mm until 270°CA and 2 mm after 270°CA. This is done because averages
in the whole domain are strongly influenced by the cooler near wall region.
In the following, the volume average of any variable ψ in the whole cylinder
will be denoted as ⟨ψ⟩_V and in the inner cylinder as ⟨ψ⟩_Vi, whereas the
average over a plane at a fixed axial position z below the cylinder head
as ⟨ψ⟩_z and the average over a plane at a fixed radial position r as ⟨ψ⟩_r.
The standard deviation of ψ will be denoted as ⟨ψ⟩_{x,rms}, where x designates

5. DNS OF THE COMPRESSION STROKE UNDER ENGINE-LIKE CONDITIONS

the volume/plane from which the standard deviation is taken from (e.g. the standard deviation in the whole cylinder is denoted as $\langle \psi \rangle_{V, \text{rms}}$). The surface average over all engine walls will be indicated as $\langle \psi \rangle_W$ and the azimuthal average as $\langle \psi \rangle_\phi$. The integral length scale $L_\psi$ is derived by first extracting $\psi$ along a circle at a fixed radial and axial position and then by integrating its autocorrelation to the point where 10% of its maximum value is reached \[124]\). The velocity magnitude will be denoted as $|v| = \sqrt{v_r'^2 + v_\phi'^2 + v_z'^2}$, while the turbulent kinetic energy is defined as $k = \frac{1}{2} (v_r'^2 + v_\phi'^2 + v_z'^2)$, where $v_r'$, $v_\phi'$ and $v_z'$ are the fluctuation velocities, $T'$ the fluctuation temperature and $Y'$ the fluctuation concentrations. The kinetic energy of the mean flow is denoted as $K E$.

5.3 Derivation of the initial conditions

In order to obtain as realistic as possible initial conditions for temperature and species fields at BDC, a separate DNS of the intake stroke was performed, which accounted for thermal and composition mixing. The velocity initial conditions were taken from the TDC of the third cycle of the cold flow simulation presented in chapter 4. Inside the cylinder the mixture is assumed to be homogeneous with $Y_{O_2} = 0.115$, $Y_{N_2} = 0.756$ and $Y_{H_2O} = 0.129$ at 900 K and atmospheric pressure. The mixture corresponds to complete combustion product of a $\varphi = 0.5$ hydrogen/air mixture and emulates EGR conditions. At the inflow a homogeneous $\varphi = 0.5$ hydrogen/air mixture at 500 K is introduced and a constant temperature of 500 K is imposed on all boundaries; for the species, zero flux boundary conditions are specified. The
5.3. Derivation of the initial conditions

Piston speed is 560 rpm and the Reynolds number based on the maximum mean jet speed, the cylinder radius and the viscosity of the intake mixture \((\nu = 4.52 \cdot 10^{-5} m^2/s)\) is \(Re = 13,643\). The Reynolds number based on the definition used in section 4.2 \((Re_{\text{max}} = V_{p,max} D_c / \nu)\) is 2,927. The initial and boundary conditions are chosen in order mimic the conditions during the intake stroke as realistic as possible.

The flow, temperature and composition fields at 11.25\(^\circ\), 90\(^\circ\) and 180\(^\circ\)CA are shown in figure 5.2. Starting from TDC the downwards moving piston draws fresh H\(_2\)/air mixture into the cylinder. At 90\(^\circ\)CA the incoming jet forms a large central cortex ring as described in section 4.4.3. The wavy structure of the jet breakup which is not observed in the incompressible flow calculation (see figure 4.8) and is related to the density gradient between the jet and the ambient fluid in the cylinder. The large central vortex ring is still visible at 180\(^\circ\)CA (indicated by a pressure iso-surface in the velocity magnitude plot with \(p_{iso} = -3.55 Pa\)). Hot EGR gases are entrained into the core of the central vortex ring, while lower temperatures can be observed close to the cylinder liner and the piston head. Visually, a correlation between the temperature and the species fields can be observed. The fields at 180\(^\circ\)CA are taken as initial conditions for the calculation of the compression stroke.

The homogeneously initialized temperature and species fields at TDC are found to have a weak effect on the conditions at the end of the compression stroke. The species are nearly homogeneously distributed at the end of the compression stroke, whereas the temperature is primarily affected by
5. DNS OF THE COMPRESSION STROKE UNDER ENGINE-LIKE CONDITIONS

Figure 5.2: Velocity magnitude, temperature and H\textsubscript{2}O mass fraction on vertical slices at 11.25°, 90° and 180°CA.

heat transfer to and from the walls and not by its initial distribution (a detailed description will be given in section 5.4).
5.4 Results and discussion

5.4.1 Evolution of the flow, temperature and composition fields during the compression stroke

The temporal evolution of the volume averaged pressure $\langle p \rangle_V$ and temperature $\langle T \rangle_V$ are shown in figure 5.3 (solid lines) and compared with the values computed for an isentropic compression using a variable specific heat capacity ratio $\gamma$. From BDC to TDC the mean temperature and pressure increase by factors of 1.93 and 23.09, respectively. This results in a reduction of the kinematic viscosity ($\nu$) by a factor of approximately 6.5, which strongly affects the evolution of turbulence, since $\nu$ is inversely proportional to the Reynolds number. The differences between DNS and the isentropic curves are very small during the first half of the compression stroke and increase significantly during the second, respectively reaching 3.9 atm and 148 K at TDC. The differences are due to the strongly increased heat transfer towards TDC, which is related to the decreasing thermal boundary layer thickness and the increasing temperature during compression. The thermodynamic loss angle is defined as the °CA difference between the peak pressure and the pressure at TDC [127,128]. In figure 5.3 the pressure curve peaks 1.54°CA before TDC, which is in the range of the thermodynamic loss angles given in the literature [128]. The relatively high heat losses are related to the low engine speed of 560 rpm and the relatively cool wall temperatures compared to the average mixture temperature at BDC.

The instantaneous flow and temperature field evolutions during the
first half of the compression stroke are illustrated in figure 5.4. At 180°CA
the flow field is dominated by a large central vortex ring in the upper half
of the cylinder [118], whose position is indicated by the yellow pressure iso-
surface. The pressure values for the iso-surfaces were chosen high enough
to capture the full vortex ring structure but low enough to select only the
locations close to the vortex core. At 202.5°CA the pressure iso-surface
becomes asymmetric and hot gases previously entrained in the vortex ring
are distributed into the whole cylinder. At 225°CA the vortex ring is still
visible but the distorted structure is followed by the disintegration of the
vortex ring at around 250°CA (not shown). The breakup of the vortex ring
structure transports the hot gases previously entrained into the vortex ring
towards the piston.

Figure 5.5 reports velocity magnitude and temperature distributions
on vertical slices at 270°, 315° and 360°CA. The pressure iso-surface is
not shown, since at 270°CA the vortex ring has almost fully disintegrated. Towards TDC the velocity magnitude decreases, as a result of the decreasing piston speed and the increasing dissipation rate. Furthermore, from 270°CA to TDC smaller length scales can be observed in $|v|$. The temperature field at 270° shows a relatively homogeneous distribution with exception of regions close to the walls. Towards TDC the thermal stratification increases significantly, which is indicated by the wider range of the color scales. This behavior is mainly related to the transport of cold gases from the boundary layer into the inner cylinder by the flow field. The same trend was also
5. DNS of the compression stroke under engine-like conditions

Figure 5.5: Temperature and velocity magnitude on slices at 270°, 315° and 360°CA.

observed in the experimental works of Dec et al. [129] and Kaiser et al. [40], where the temperature fields in ICEs were measured on planar slices using LIF. The origin of the increasing thermal stratification will be discussed in detail in section 5.4.4.

Figure 5.6 shows the evolution of the azimuthally averaged velocity magnitude in the axial and radial directions ($|v|_{z,r} = \sqrt{v_r^2 + v_z^2}$) during the compression stroke. The azimuthal average of the azimuthal velocity is not considered, since it is always close to zero. At BDC the piston speed is zero and $\langle |v|_{z,r} \rangle_\phi$ is dominated by the large central vortex ring in the upper half of the cylinder. At 225°CA the piston moves upwards with a speed of 0.88 $m/s$
imposing a flow in the axial direction. Compared to BDC the vortex ring size and strength are reduced and the vortex ring center is pushed upwards. The mean flow field at $270^\circ$CA is dominated by the axial velocity imposed by the piston. The remains from the vortex ring are still visible but the flow speed around the vortex ring core is lower compared to the piston velocity. In addition, the spatial extend is restricted to the edge between cylinder head and liner. After $270^\circ$CA the piston decelerates resulting in decreasing mean velocities, which are significantly lower compared to the instantaneous velocities shown in figure 5.5. At TDC the piston velocity and accordingly the mean flow velocities are close to zero.

The azimuthally averaged temperature distributions $\langle T \rangle_\phi$ during compression are plotted in figure 5.7. The increased temperatures close to the
cylinder head at BDC are attributed to hot gases entrained in the vortex ring. After the disintegration of the vortex ring the hot gases are distributed in the whole cylinder, resulting in a relatively uniform temperature in the bulk gas at 270°CA. At 306°CA the hottest zone is located in the cylinder center, while relatively lower temperatures can be observed close to the cylinder liner.

The values of $k$, $KE$, $\varepsilon$, $T_{rms}$ and $\langle Y \rangle_{V,rms} / \langle Y \rangle_{V}$ at different °CA during the compression stroke are reported in table 5.2. The decreasing kinematic viscosity results in higher velocity gradients around the smaller flow structures, and thus in increased dissipation during compression. The peak in $\varepsilon$ is reached at 346°CA (i.e. before TDC), so that close to TDC the turbulent kinetic energy is strongly reduced by the high dissipation level.
The kinetic energy based on the mean velocities is during the first half of the compression stroke approximately 2 to 3 times smaller compared to $k$. With decreasing piston speed towards TDC, $KE$ decreases significantly, resulting in $k/KE \approx 9$ at TDC. The relatively low mean flow velocities are attributed to the unstable vortex ring, which transforms kinetic energy of the mean flow into turbulence. Significantly higher $KE/k$ ratios ($KE/k \approx 2$ at ignition timing) are reported for a tumbling intake configuration in the dissertation of Buschbeck [130]. This may be due to the relatively stable tumble flow, which stores the mean kinetic energy introduced during the intake stroke. In addition, the PIV measurements were performed on a slice on the symmetry plane, where the tumble flow reaches its maximum strength. If the flow field is measured on slices at different locations the $KE/k$ ratio can differ significantly.

As shown in Hawkes et al. [56], temperature fluctuations can affect the autoignition time and pressure peak in a HCCI type combustion mode significantly. The temperature fluctuations drop from BDC to 225°CA but increase significantly after 270°CA, mainly as a result of the increasing difference between the average temperature in the cylinder and the fixed wall temperatures. This behavior is in agreement with the LIF measurements of Snyder et al. [37] and Kaiser et al. [40]. Since the mixture is more likely to autoignite inside the hotter inner cylinder zone, a more useful quantity for the description of thermal stratification is the average temperature fluctuations in the inner cylinder $\langle T \rangle_{V_i,rms}$. This quantity decreases from 12.20 to 6.81 K during the first half of the compression stroke, possibly due to the
5. DNS of the compression stroke under engine-like conditions

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<th>$\langle k \rangle_V$</th>
<th>$\langle KE \rangle_V$</th>
<th>$\langle \varepsilon \rangle_V$</th>
<th>$\langle T \rangle_{V,rms}$</th>
<th>$\langle T \rangle_{V_i,rms}$</th>
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<td>36641.3</td>
<td>110.7</td>
<td>39.15</td>
<td>0.010</td>
</tr>
<tr>
<td>360</td>
<td>0.98</td>
<td>0.11</td>
<td>25510.0</td>
<td>119.9</td>
<td>47.31</td>
<td>0.009</td>
</tr>
</tbody>
</table>

Table 5.2: Variation of $\langle k \rangle_V$, $\langle KE \rangle_V$, $\langle \varepsilon \rangle_V$, $\langle T \rangle_{V,rms}$, $\langle T \rangle_{V_i,rms}$ and $\frac{\langle Y_{H_2O} \rangle_{V,rms}}{\langle Y_{H_2O} \rangle_V}$ during compression (in $m^2/s^2$, $m^2/s^3$, $K$).

homogenization of the temperature field in the inner cylinder. The trend reverses during the second half and the significant increase of $\langle T \rangle_{V_i,rms}$ is related to the strongly enhanced wall heat transfer towards TDC.

The species mixing is analyzed using the ratio of the standard deviation of $Y_{H_2O}$ and the average water vapor concentration. $\langle Y \rangle_{V,rms} / \langle Y \rangle_V$ reduces from 17.4 % at BDC to 3.3 % at piston half way up (270°CA) indicating a very efficient mixing process. At TDC the mixture is nearly homogeneously distributed.

The probability density functions ($PDF$s) of turbulent kinetic energy and temperature within the whole cylinder are plotted in figure 5.8 for several piston positions. At 180°CA the $PDF(k)$ shows a relatively flat profile with a peak at approximately 0.73 $m^2/s^2$. During compression the peak becomes more pronounced but the position of the maximum remains at values close to 0.7 $m^2/s^2$. The relatively large difference in the peak values at 346° and 360°CA can be attributed to the increased dissipation rate
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towards TDC. According to Luong et al. [60] the direct effect of velocity fluctuations on autoignition is small compared to the effect of thermal stratification. Hence, the flow is indirectly influencing autoignition by enhancing thermal stratification due to convective heat transport close to walls.

The influence of the initial conditions on temperature can be seen by comparing the $PDF(T)$ at $180^\circ$ and $225^\circ$CA. The minimum and maximum temperatures are similar but the peak becomes more pronounced and shifts to a higher value, as a result of the temperature homogenization during the early compression stage discussed above. The higher peaks at $225^\circ$ and $270^\circ$CA are due to the low temperature fluctuations in the inner cylinder (table 5.2). The steep gradients on the right side of the PDFs between $225^\circ$ and $306^\circ$CA indicate that at these times the temperatures in the inner cylinder are almost not influenced by the relatively cooler boundary layer. The $PDF$ shape differs significantly from the almost Gaussian distribution reported in the experimental study of Kaiser et al. [40], possibly because of the difficulty in resolving the thermal boundary layers using two-dimensional measurements.

Between $306^\circ$ and $333^\circ$CA the maximum $PDF(T)$ values decrease strongly, due to the increased entrainment of cold boundary layer gases into the inner cylinder. Close to TDC ($346^\circ$ and $360^\circ$CA), the $PDF(T)$ becomes almost flat indicating that also fluid in the inner cylinder is strongly influenced by the wall heat losses. The maximum temperature 1234.5 $K$ is reached at $360^\circ$CA although the average temperature is nearly the same as at $346^\circ$CA (table 5.2). The temporal development of $PDF(T)$ indicates
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Figure 5.8: Probability density functions of (a) turbulent kinetic energy and (b) temperature at several piston positions during compression.

that the temperature initial conditions are washed out after the first half of the compression stroke, implying that, at least for this setup, the thermal stratification at TDC cannot be controlled by changing the temperature field at BDC. Stronger effects can be expected by modifying the wall temperature, as reported in Sjöberg et al. [131], where it was found that lower coolant temperature has a strong effect on the heat release rate for HCCI operation.

5.4.2 Behavior at TDC

The initial and boundary conditions of the compression stroke are chosen in order to reach auto igniting conditions shortly before TDC. The combustion process after ignition will be strongly influenced by the fluctuations in the velocity, temperature and composition fields.

Figure 5.9 reports distributions of the velocity magnitude, temperature, $Y_{H_2O}$ and $v'_z$. The velocity magnitude and $v'_z$ varies strongly in the
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domain and no large scale structures can be identified. The temperature field shows high fluctuations in the whole domain with steep gradients close to the cylinder wall. In the inner cylinder region temperatures below 1050 K and above 1200 K can be observed, with the average temperature being close to 1110 K. As discussed in Hawkes et al. [56] high temperature fluctuations have a strong effect on autoignition timing and peak pressure in a compression ignition combustion mode. The origin of the fluctuations will be discussed in section 5.4.4. The water vapor is almost homogeneously distributed inside the cylinder, as indicated by the narrow range of the color scale, which is in agreement with table 5.2.

The PDFs and the average values of the radial and azimuthal fluctuation velocities reported in figure 5.10 are nearly identical, while the average in axial direction \( \langle |u'_z| \rangle \) is approximately 25% lower. Accordingly, the peak PDF value is increased possibly due to the dumping of axial fluctuations in the narrow gap between piston and cylinder head.

In figure 5.11 the integral length scale distributions of \( k \) and \( T \) are plotted on a vertical slices. Values close to the cylinder center are not shown, since in this region the number of statistically independent points is too low to obtain meaningful values. With the exception of two zones close to the cylinder head, \( L_k \) lies in the range between 1 and 2.5 mm. \( L_T \) varies between 3 and 4 mm in the cylinder center and decreases towards the walls due to increased temperature fluctuations in the thermal boundary layer. The reduced length scales are related to an in average cooler temperature at the walls, which result in reduced kinematic viscosity. Overall, the average
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| Temperature [K] | $|\mathbf{U}|$ [m/s] | $Y_{H2O}$ | $|\mathbf{U}'_z|$ [m/s] |
|-----------------|-----------------|----------|-----------------|
| 1225            | 3.36            | 3.25e-2  | 3.04e-2         |
| 900             | 3.04e-2         | 3.25e-2  | 2.8             |
| 0               | 2.8             | 3.25e-2  | 0               |

Figure 5.9: Velocity magnitude, temperature, $Y_{H2O}$ and $v'_z$ distribution on a horizontal slice at $z = -3.75$ mm at TDC.

Figure 5.10: PDF of the axial, radial and azimuthal fluctuations velocity components at TDC.
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Figure 5.11: Integral length scales [mm] of the turbulent kinetic energy and the temperature at TDC.

The length scale of \( k \) is approximately 25% smaller compared to the average scale of the temperature.

The PDFs of \( L_k \) and \( L_T \) plotted in figure 5.12 have a similar shape and their peaks are located at approximately 1.1 mm. In contrast, \( PDF(\eta_k) \) is more symmetric and \( \eta_k \) ranges from 0.005 to 0.025 with an average value of 12.8 \( \mu \)m. The smaller \( \eta_k \) values are mainly located in the relatively cooler thermal boundary layers since \( \nu \propto T^{1.5} \). In Heim and Ghandhi [132] the Kolmogorov scale at TDC of the compression stroke was estimated by adjusting model spectra based on PIV data. According to [120] the model spectra is defined as \( E(\kappa) = 1.5\varepsilon^{2/3}\kappa^{-5/3}f_Lf_\eta \), where \( \kappa \) is the wave number and \( f_L \) and \( f_\eta \) are non-dimensional functions. The parameters in the \( E(\kappa) \) were then derived using the definition of the turbulent Reynolds-number and the PIV results.

The investigated engine has a compression ratio of 10 and different turning speeds and intake port configurations are investigated. For a turn-
5. DNS of the Compression Stroke under Engine-Like Conditions

Figure 5.12: PDF of the integral length scales of turbulent kinetic energy, temperature and the Kolmogorov scale at TDC.

Engaging speed of 600 rpm Kolmogorov scales between 17.4 and 25.9 μm were reported. This agrees well with the 12.8 μm obtained in this work when differences in the compression ratio are taken into consideration (12 instead of 10). The ratio between \( \langle L_k \rangle_V \) and \( \langle \eta_k \rangle_V \) at TDC is approximately 161. The low value of \( \langle \eta_k \rangle_V \) close to TDC is mainly due to the increasing pressure, which results in a reduced kinematic viscosity and a higher dissipation rate. On the other hand, the influence of the increasing temperature on \( \langle \eta_k \rangle_V \) is less pronounced, since temperature is less sensitive to volume changes compared to pressure.

5.4.3 Velocity and thermal boundary layer

The velocity and thermal wall boundary layers are investigated on the cylinder head for \( r/r_c < 0.9 \), since outside this region the boundary layers of the liner interacts strongly with that from the cylinder head. The boundary lay-
ers are found to be very similar at all engine walls (cylinder head, liner and piston). The reason for the small differences at the cylinder liner compared to cylinder head and piston are discussed in section 5.4.3.5.

5.4.3.1 Velocity boundary layer

As described in section 5.4.1 the mean flow varies significantly in time and space and the mean kinetic energy is small compared to the turbulent kinetic energy. Thus, the wall shear stress cannot be calculated based on mean velocity gradients and accordingly the wall local shear stress \( \tau_W \) is defined in this work as:

\[
\tau_W = \sqrt{\tau_{wx}^2 + \tau_{wy}^2 + \tau_{wz}^2}.
\]  

(5.1)

where \( \tau_{wx} = \mu \left( \frac{\partial v_y}{\partial x} \right)_W \), \( \tau_{wy} = \mu \left( \frac{\partial v_y}{\partial y} \right)_W \) and \( \tau_{wz} = \mu \left( \frac{\partial v_z}{\partial z} \right)_W \) are calculated based on the viscosity and instantaneous velocity gradients at the walls. The scalar \( \tau_W \) value is derived by averaging over the considered surface (i.e. the segment of the cylinder head). The definition of \( \tau_W \) in this work differs from the one commonly used in the literature, where \( \tau_W \) is calculated based on the mean velocity gradient. This has to be taken into account when comparing the results of this work with the literature. Relative comparisons during the compression stroke are directly possible, since in this work always the same definition for \( \tau_W \) is used.

Figure 5.13(a) shows the variation of the average velocity magnitude with increasing distance from the cylinder head at several times during the compression stroke. According to Johnston and Flack [133] the velocity magnitude \( |v| \) is used instead of the mean velocity in the streamwise di-
rection $U$, since no steady mean flow in the wall parallel direction can be observed in the flow field. In agreement with the definition of $\tau_W$, $|v|$ is calculated based on instantaneous velocities. During compression increasing velocity gradients are observed at the walls, as a result of the decreasing kinematic viscosity. Exceptions are the relatively steep gradient at $225^\circ$CA, which is connected to the central vortex ring shown in figure 5.6, and the reduced gradient at $360^\circ$CA, which can be attributed to the reduction of the turbulent kinetic energy towards TDC (table 5.2).

According to Huang et al. \cite{81} two definitions for the transformation from physical into wall-normal units can be used. In the classical definition $y^+ = \frac{y}{\nu W} \sqrt{\frac{\tau W}{\rho W}}$, $\rho_W$ and $\nu_W$ are defined at the engine walls, where a fixed temperature of 500 K has been imposed. On the other hand, for the semi-local scaling $y^* = \frac{y}{\nu(y)} \sqrt{\frac{\tau W}{\rho(y)}}$, $\rho(y)$ and $\nu(y)$ are defined at the local temperature at the actual wall distance $y$. In the following the semi-local scaling will be denoted as $y^*$ and the classical scaling as $y^+$. The dashed lines in figures 5.13(b) and (c) represent the law-of-the-wall defined as \cite{134}: 

$$u^+ = \begin{cases} y^+ & : y^+ < 10 \\ 1/\kappa \ ln(y^+) + B & : y^+ > 10 \end{cases}$$

the constants $\kappa$ and $B$ are according to Pope \cite{120} for channel flows within 5\% of $\kappa = 0.41$ and $B = 5.2$.

Figure 5.13(b) shows the non-dimensional velocity profiles based on the classical scaling. In the viscous sublayer ($y^+ < 5$) the non-dimensional average mean velocity profiles follow the line $u^+ = y^+$ at all times during
the compression stroke. Further away from the wall \((y^+ > 8)\), the \(\langle |v| \rangle_z^+\) curves start to deviate from each other and increasing \(\langle |v| \rangle_z^+\) values for curves closer to TDC can be observed. This behavior is in agreement with the observations reported in Jainski et al. \cite{Jainski2017} (see section 2.3.1).

In figure 5.13(c) the non-dimensional velocity profiles are plotted using the semi-local scaling, which takes the influence of the local temperature on density and viscosity into account. In contrast to the classical scaling, the curves calculated based on the semi-local scaling collapse also in the buffer and the log-law region. According to Huang et al. \cite{Huang2017} and Nicoud \cite{Nicoud2017} this indicates that the differences in figure 5.13(b) can be mainly attributed to density variations in the boundary layer.

The agreement of the wall-normal velocity profiles with the \(|v|^+ = y^+\) curve for \(y^+ < 5\) shows that the statistics based on instantaneous velocities lead to similar results compared to the statistics based on mean flow velocities. This is plausible, since in the viscous sublayer the flow is mainly influenced by viscosity. The deviations from the law-of-the-wall in the buffer and log-law region \((y^+ > 8)\) are difficult to interpret, since the mean flow differs significantly from a steady channel flow and \(\tau_W\) is defined differently.

According to Tennekes and Lumley \cite{Tennekes1972}, the relation:

\[
\langle u \rangle / \langle u \rangle_{rms} = c \ln(y) + d
\]

(5.2)

is necessary for the existence of a logarithmic velocity profile. The relationship is independent from the wall shear stress \((\tau_W)\) and is expected also to

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Figure 5.13: (a) Mean velocity magnitude vs. distance from the cylinder head; $|v|^+$ vs. $y^+$ with (b) classical and (c) semi-local scaling.

be valid for the velocity magnitude, since according to Nicoud [82] the velocity fluctuations in the log-law region are significantly lower compared to the mean velocity. Thus, the relation will be used to assess if the law-of-the-wall can describe the boundary layer in this setup.

In figure 5.14, the ratio $\langle |v| \rangle _z / \langle |v| \rangle _{z,rms}$ is plotted versus $ln(y)$ at several times during the compression stroke. In the viscous sublayer similar gradients and shapes can be observed at all times, while significant deviations are visible in the log-law region. Thus, in this case a constant slope cannot accurately describe the velocity profiles in the log-law region. This observation agrees well with the results reported in Jainski et al. [2], who also report the velocity boundary layer based on the relation of Tennekes and Lumley [135]. A possible explanation for the deviation is the different mean flow field, since in Hattori and Nagano [86] in an impinging jet setup depending on the mean flow direction significant deviations from the law-of-the-wall are reported.

The dimensional radial velocity fluctuations as function of the distance
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Figure 5.14: $\langle |v| \rangle_z$ devided by $\langle |v| \rangle_{z,rms}$ versus $\ln(y)$; from the wall are plotted in figure 5.15(a). During compression increasing gradients at the wall can be observed, which are related to the decreasing kinematic viscosity. The relatively high radial fluctuation velocities at 225°CA are related to the large central vortex ring and the reduced fluctuation velocities at TDC can be attributed to the lower turbulent kinetic energy (table 5.2).

When plotted with respect to the classical and semi-local scaling (figure 5.15(b) and (c)) the curves collapse in the viscous sublayer during the compression stroke. The semi-local scaling shown in figure 5.15(c) results in a narrower range compared to the classical scaling but the curves do not overlap at $y^* = 100$. The behavior of the radial fluctuation velocities in figure 5.15(c) agrees well with the results reported in the computational study of Nicoud [82], where an improved agreement of the radial velocity fluctuations for different temperature ratios using the semi-local scaling was
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Figure 5.15: (a) Radial velocity fluctuations $\langle v_r \rangle_{z,\text{rms}}$ vs. distance from cylinder head; $\langle v_r \rangle_{z,\text{rms}}^+$ vs. $y^+$ with (b) classical scaling and (c) semi-local scaling.

The profiles of the velocity fluctuations in the azimuthal direction (figure 5.16) are, with the exception of the one at 225°CA, similar to the velocity fluctuations in the radial direction. Close to the cylinder wall the large central vortex ring imposes mainly velocities in the radial and axial directions and thus has only a limited effect on the velocity fluctuations in the azimuthal direction. Accordingly, the azimuthal velocity fluctuations at 225°CA are less influenced by the vortex ring, since the mean flow in the azimuthal direction is close to zero during the whole compression stroke.

In figure 5.17(a) $\langle v_z \rangle_{z,\text{rms}}$ is plotted versus distance from the cylinder head. In contrast to figures 5.15 and 5.16, the range of the wall distance is extended to 5 mm (corresponding to $y^+ = 200$ in wall-normal units), since the gradients at the walls are significantly smaller. With the exception of 360°CA, the gradients at the cylinder head increase towards TDC. Compared to $\langle v_r \rangle_{z,\text{rms}}$ and $\langle v_\varphi \rangle_{z,\text{rms}}$ the fluctuations in the axial direction
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Figure 5.16: (a) Azimuthal velocity fluctuations $\langle v_\phi \rangle_{z, \text{rms}}$ vs. distance from cylinder head; $\langle v_\phi \rangle^+_{z, \text{rms}}$ vs. $y^+$ with (b) classical scaling and (c) semi-local scaling.

Figure 5.17: (a) Axial velocity fluctuations $\langle v_z \rangle_{z, \text{rms}}$ vs. distance from cylinder head; $\langle v_z \rangle^+_{z, \text{rms}}$ vs. $y^+$ with (b) classical scaling and (c) semi-local scaling.

increase significantly slower, which can be attributed to the dampening effect of the wall [120]. In figures 5.17(b) and (c) the wall normal velocity fluctuations are plotted in wall-normal coordinates with respect to the classical and semi-local scaling, respectively. Both plots depict a similar collapse of the curves during compression. This agrees with the observations of Nicoud [82], reporting a more pronounced collapse for the wall normal velocity fluctuations in comparison to the wall parallel velocity fluctuations.
According to Tennekes and Lumley [135], a mean velocity is required for the creation of shear stresses. As described in section 5.4.1, the mean velocities are relatively low and thus in the current setup profiles of all shear stresses are close to zero. This applies for the cylinder wall as well, since the piston-induced axial velocities during the compression stroke are too low for the formation of high shear stress components at the cylinder wall.

5.4.3.2 Thermal boundary layer

Planar averaged temperature profiles \( \langle T \rangle_z \) are plotted versus the distance from the cylinder head in figure 5.18(a). The temperature gradients at the cylinder head and temperatures at 3 \( mm \) distance to the cylinder head increase towards TDC. For all piston positions the high gradients flatten out with increasing distance from the wall and at around 1 \( mm \) the profiles become nearly horizontal.

The temperature evolution in wall-normal units are plotted in figure 5.18(b) with classical and 5.18(c) with semi-local scaling. In addition, the thermal law-of-the-wall in the viscous sublayer is shown in the graphs and is calculated by the following equation [136]:

\[
T^+ = \begin{cases} \frac{Pr y^+}{2.075 \ln(y^+)} + 3.9 & : y^+ < 10 \\ Pr y^+ & : y^+ > 30 \end{cases}
\]

The thermal law-of-the-wall for \( y^+ > 30 \) is not shown in figures 5.18(b) and (c), since it is outside the range of the axis scaling. Temperature is transformed into wall-normal units using \( \langle T \rangle_z^+ = (T_W - T) \rho_W c_p u_r / q_W \).
where \( T_W \) is the temperature at the wall, \( c_p \) the heat capacity at the wall, \( u_\tau \) the friction velocity and \( q_W \) the heat flux. In the viscous sublayer the \( \langle T \rangle^+ \) profile agrees well with the thermal law-of-the-wall. In the buffer and log-law regions the temperature profiles deviate from the thermal law-of-the-wall and tend to increase towards TDC. With the use of the semi-local scaling (figure 5.18(c)) a collapse of the curves during compression can be observed, which is in agreement with the findings in Huang et al. [81] and Nicoud [82]. This suggest that comparable to the flow field the differences during compression in figure 5.18(b) are mainly due to density variations.

The temperature profiles in figures 5.18(b) and 5.18(c) are similar compared to Hattori and Nagano [86], where the boundary layer in an impinging jet setup is investigated. This indicates that the thermal boundary layer is strongly influenced by the mean velocity field which explains the deviation from the thermal law-of-the-wall, since it violates the assumption of a steady wall-parallel flow.

Figure 5.19(a) plots the temperature fluctuations in dimensional form.
versus the wall distance. A clearly defined maximum, whose position shifts
towards the wall with time can be seen, with a peak increasing from 30 K
at 225°CA to 125 K at TDC. The temperature fluctuations further away
from the wall (distance > 2 mm) are also increasing towards TDC (see also
table 5.2).

The temperature fluctuations in classical wall-normal coordinates are
plotted in figure 5.19(b). Close to the wall ($y^+ < 5$) a collapse of all curves
can be observed but the peak values differ significantly during compression.
The relatively high $\langle T \rangle_{z,\text{rms}}^+$ peak value at 225°CA can be attributed to the
vortex ring illustrated in figure 5.4. This behavior gives an indication of the
influence of large scale flow structures on temperature stratification. The
peak location of $\langle T \rangle_{z,\text{rms}}^+$ varies between approximately $y^+ = 7.5$ at 225°CA
and $y^+ = 12.5$ at 360°CA. Compared to channel flow DNS calculations [80],
[137] and [126], where the peaks are located at $y^+ \geq 20$, the peaks in this
work are located closer to the wall. The peak values of $\langle T \rangle_{z,\text{rms}}^+$ are slightly
below the maximum values reported in the literature [80], [137], [126], which
are commonly $\langle T \rangle_{z,\text{rms}}^+ > 2$. These differences may be due to the different
definition of $\tau_W$.

When plotted with respect to the semi-local scaling (figure 5.19(c)) a
clear reduction of the relative differences of peak heights and positions can
be seen, which agrees with the velocity field and with the observations in
Nicoud [82].
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Figure 5.19: (a) \( \langle T \rangle_{z,rms} \) vs. distance from cylinder head; \( \langle T \rangle^+_{z,rms} \) vs. \( y^+ \) with (b) classical and (c) semi-local scaling.

5.4.3.3 Correlation between the velocity and thermal boundary layers

The correlation between wall-normal velocity and temperature is important for wall heat transfer, since it appears in the convective term of the total heat flux equation, which according e.g. to Nicoud \[82\] in one-dimension becomes:

\[
q = -\rho c_p \langle v' T' \rangle + \lambda \frac{\partial T}{\partial x} \quad (5.3)
\]

where \( v' \) and \( T' \) are the velocity and temperature fluctuations and \( \frac{\partial T}{\partial x} \) the temperature gradient in direction \( x \).

In figure 5.20(a), \( \langle v' T' \rangle_z \) is plotted versus wall distance in dimensional form. With increasing distance the slopes and maximum values increase with time, reaching a peak at locations between 0.38 and 1.5 \( mm \) away from the cylinder head and decrease farther away from the wall. Towards TDC the peak heights increase and the position shifts closer to the wall. The relatively lower peak value at TDC can be attributed to the reduced turbulence as the piston approaches the cylinder head.
In wall-normal units with respect to the classical scaling (figure 5.20(b)) all curves collapse for $y^+ < 10$, indicating a similar correlation during the compression stroke. For $y^+ > 10$ the curves deviate from each other resulting in a peak value of 0.6 at 270°CA which increases to 1.28 at TDC. With respect to the semi-local scaling (figure 5.20(c)), a nearly full collapse of the curves can be observed, indicating a similar non-dimensional correlation between temperature and wall-normal velocity fluctuations during the whole compression stroke. The maximum values and the non-dimensional wall distance of the peaks are in range of the maxima reported in the numerical channel flow investigations of Araya et al. [126] and Kong et al. [137], especially when using the semi-local scaling (5.20(b)). However in the impinging jet setup studied by Hattori et al. [86] large variations in the $\langle v_z' T' \rangle^+_z$ profiles depending on the local mean flow are reported and thus comparisons between different flow types are difficult.
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5.4.3.4 Boundary layer thickness

A clear definition of the wall boundary layer thickness is difficult, since in this case in contrast to channel or pipe flows a clearly defined mean flow velocity outside the boundary layer \( u_\infty \) does not exist. Thus, the commonly used definitions reported in e.g. Schlichting [138] cannot be used. In the following, the boundary layer thickness is defined based on the velocity and temperature gradients. As reported in sections 5.4.3.1 and 5.4.3.2 the gradient of the temperature and velocity profiles decreases with increasing wall distance. The boundary layer thickness is then defined by the position where the maximum gradient at the wall is reduced to an arbitrary threshold percentage. The threshold value is varied in a broad range between 50\% and 90\%, in order to estimate the impact of chosen threshold value.

The resulting flow and temperature boundary layer thicknesses are shown in figures 5.21(a) and (b). With varying thresholds the relative trend during compression remains unaffected. The boundary layer thicknesses of flow and temperature are comparable and show the same relative trends during compression. The observed trend of the boundary layer thickness agrees well with Jainski et al. [2], where also reduced boundary layer thickness close to TDC are reported.

5.4.3.5 Boundary layer at the cylinder liner

The axial mean flow imposed by the moving piston (section 5.4.1) is at the liner directed parallel to the wall, which is in contrast to the cylinder
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Figure 5.21: (a) Flow boundary layer thickness with varying threshold values; (b) thermal boundary layer thickness with varying threshold values.

head and the piston. The influence of the axial mean flow on the velocity boundary layer at the cylinder liner is investigated in figure 5.22 by comparing the axial (solid lines) with the azimuthal velocity fluctuations (dashed lines). The standard deviation is taken on surfaces with constant radii and thus constant distance from the cylinder liner. Distances of 7.5 mm (until 270°CA) and 2 mm (after 270°CA) from the cylinder head and piston are not considered, since they overlap with the boundary layers from the cylinder head and the piston.

At 270°CA, the highest deviation between the fluctuations in the azimuthal and axial directions can be observed, since at this time the piston velocity reaches its maximum. In a channel flow the ratio of the peak velocity fluctuations in the streamwise and spanwise directions are typically above 2.5 (see, for example in Kim et al. [78]), which is significantly higher compared to the ratio of approximately 1.5 obtained here. Thus, the influence of the mean axial velocity on the boundary layer at the cylinder liner
is significantly less pronounced compared to channel or pipe flows even at the time of the maximum piston speed. After 333°CA the axial mean flow is significantly reduced resulting in similar velocity fluctuations in the axial and azimuthal directions.

Figure 5.23 shows the velocity magnitude (a) and temperature (b) profiles in semi-local wall-normal units at the cylinder wall. Compared to the profiles at the cylinder head (figures 5.13(c) and 5.18(c)) only marginal differences can be observed, indicating that the boundary layer structure is similar for all engine walls.
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5.4.4 Wall heat transfer

5.4.4.1 Global wall heat transfer

The evolution of the mean heat flux \( \langle q_W \rangle \) during compression is plotted in figure 5.24(a), where \( q_W \) is calculated as:

\[
q_W = \lambda \frac{\partial T}{\partial n} \tag{5.4}
\]

with \( \frac{\partial T}{\partial n} \) being the temperature gradient in wall normal direction \( n \) and \( \lambda \) the thermal conductivity. The values are calculated at six selected piston positions (circle markers) and the red line is a cubic interpolated spline. Positive values are defined as energy transferred out of the system boundaries.

At BDC the mean heat flux is close to zero, since the temperature difference between wall (500 K) and fluid in the cylinder is relatively small. Until 306°CA (approximately 70% of the compression time) the mean heat flux increases moderately to 0.062 MW/m². After 306°CA the slope increases.

Figure 5.23: (a) \( \langle |v| \rangle_\tau^* \); (b) \( \langle T \rangle_\tau^* / Pr \) vs. \( y^* \) with semi-local scaling.
fast to the maximum mean heat flux of approximately 0.265 MW/m². The
subsequent decrease close to TDC can be attributed to the reduction in
turbulent kinetic energy (table 5.2). When comparing the shape of the
mean heat flux curve with the temperature and pressure evolutions (figure
5.3), the pressure curve shows a qualitatively higher correlation (strong in-
crease close to TDC). At first, this may be surprising, since the heat flux
\( q_w = \lambda \frac{\partial T}{\partial n} \) is calculated based on the temperature gradients (\( \frac{\partial T}{\partial n} \)) and
the pressure has a negligible influence on thermal conductivity (\( \lambda \)) for the
considered conditions. The reason for this behavior is the increasing den-
sity, which results in a decreasing kinematic viscosity and thereby higher
temperature gradients at the wall. Figure 5.24(b) plots the total heat loss,
calculated by the product of the engine surface area and the mean heat flux.
Due to the decreasing surface area during compression the relative increase
of the total heat loss is lower compared to the mean wall heat flux. The
maximum heat loss of 2760 W is reached shortly before TDC.

The ratio between the maximum turbulent heat fluxes (\( q_{t,\text{max}} \)) and the
wall heat fluxes are investigated in table 5.3. The maximum turbulent heat
flux is calculated by the following equation:

\[
q_{t,\text{max}} = \rho(y) c_p(y) \left< v_z' T' \right>_{z,\text{max}} \quad \text{(5.5)}
\]

where \( \rho(y) \) and \( c_p(y) \) are the density and specific heat capacity at the thermodynamic conditions at the peak position of \( \left< v_z' T' \right>_{z,\text{max}} \) close to the wall
(figure 5.20(a)). In general for the observed setup between 60% and 80%
of the heat flux at the cylinder head are related to turbulent heat fluxes.
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![Graphs](image)

Figure 5.24: (a) Average heat flux over all engine walls; (b) total heat loss through all engine walls.

The decreasing ratio between 225° and 270°CA is possibly related to the increasing piston speed. With decelerating piston speed the ratio increases to 76% towards TDC. The work of Sakakibara et al. [139] determined the turbulent heat fluxes in the stagnation region of a water jet impinging at a flat wall. In this configuration around 20% of the heat flux are supplied by turbulent fluctuations. The difference to this work can be attributed to the different flow field, since according to Hattori and Nagano [86] the turbulent heat flux depends strongly on the mean velocity. Close to the stagnation point very low maximum turbulent heat fluxes are reported which with increasing distance from the impingement center increase significantly. In addition, the spatial PIV resolution of 1 mm in [139] is very coarse for an investigation of the boundary layer structure.

In the following the evolution of the heat transfer coefficient ($\alpha$) defined
5.4. Results and discussion

\[
\alpha = \frac{\langle q_w \rangle_W}{\langle T \rangle_V - T_W} \tag{5.6}
\]

is analyzed in detail. In equation (5.6) \( \langle T \rangle_V \) is the cylinder averaged temperature and \( T_W \) the wall temperature. In figure 5.25(a) it can be seen, that the heat transfer coefficient increases from approximately 78 W/m²K at 225°CA to the maximum value of approximately 470 W/m²K shortly before TDC. The increase of \( \alpha \) during compression can be attributed to the decreasing kinematic viscosity, leading to decreasing minimum length scales in the flow and temperature fields and hence increased velocity and temperature gradients at the engine walls (section 5.4.3). The reversing trend between 346° and 360°CA can be explained by the significantly reduced turbulent kinetic energy at TDC (table 5.2) which is followed by decreasing turbulent heat fluxes towards the wall (figure 5.20).

The heat transfer coefficients extracted from the DNS is compared to the global 0D wall heat transfer models of Woschni [5] and Hohenberg [6] (equations (2.1) and (2.2)). The heat transfer coefficients of the global models were calculated with the standard constants for non-swirling flows using the pressure and temperature from the DNS calculation. The heat transfer coefficient based on the Hohenberg correlation agrees qualitatively reasonable well with the DNS data but underpredicts \( \alpha \) by approximately 50 - 100

<table>
<thead>
<tr>
<th>°CA</th>
<th>225</th>
<th>270</th>
<th>306</th>
<th>333</th>
<th>346</th>
<th>360</th>
</tr>
</thead>
<tbody>
<tr>
<td>( q_{t,max}/q_w \times 100 )</td>
<td>78.1</td>
<td>62.1</td>
<td>62.0</td>
<td>70.8</td>
<td>72.09</td>
<td>76.0</td>
</tr>
</tbody>
</table>

Table 5.3: Ratio between the maximum turbulent heat flux and the wall heat transfer.
5. DNS of the compression stroke under engine-like conditions

\[ W/m^2K \] during the compression stroke. The trend reversal between 350° and 360°CA is not predicted by the correlation. The Woschni correlation on the other hand underpredicts the heat transfer coefficient significantly during the whole compression stroke. Similar observations were made in the experimental works of Chang et al. [89] and Mollenhauer [140], which report an underprediction of the Woschni-model during the compression stroke for low engine speeds. However, a direct comparison between DNS and experiments is difficult, since for the in-cylinder pressure analysis the model constants of the global models are adjusted in order to satisfy the global energy balance. In addition, the Woschni and Hohenberg models are designed for real engine applications including additional effects like soot particles at the walls which can have an impact on the wall heat transfer coefficient.

Figure 5.25(b) shows the Probability Density Functions (PDF) of the local heat transfer coefficients at several piston positions over all engine walls. During compression the peaks are reduced and the peak position shifted towards higher heat transfer coefficients. The reversing trend between 346° and 360°CA can be explained by the reduced turbulent heat flux (figure 5.20). The gradient on the left side of the maximum is in all curves significantly higher compared to the gradient on the right side. This is related to the near wall flow behavior in case the flow moves towards the wall, as will be discussed in section 5.4.4.3. The transfer coefficients close to zero are located on the cylinder edges.
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Figure 5.25: Heat transfer coefficients versus the piston position of the DNS calculation and the correlations from Woschni [5] and Hohenberg [6].

Figure 5.26: Wall heat flux distribution through the cylinder head at 270°, 306° and 360°CA.

### 5.4.4.2 Local distribution of the wall heat transfer

Instantaneous heat flux distributions on the cylinder head at 270°, 306° and 360°CA are shown in figure 5.26. Towards TDC the size of the heat flux structures is significantly reduced. Regions with on average higher heat fluxes exhibit high fluctuations, while more uniform heat flux distributions are observed in zones with in average lower heat fluxes.
In order to quantify the evolution of the size of the heat flux structures in figure 5.27 the integral length scales of $q_W$ at the cylinder head are plotted with respect to the piston position. The shown values are averaged out of 40 individual integral length scales, which are computed on circles with radii between $r/r_c = 0.5$ and 1. The region close to the cylinder center ($r/r_c < 0.5$) is not considered, since the number of statistically independent samples is too small to derive converged statistics (see appendix A.1). During compression $L_{qW}$ decreases from approximately 2.75 mm at 225°CA to below 0.75 mm at TDC. The reduced length scales imply for wall resolved engine LES simulations that in addition to mesh refinements normal to the wall (see figure 5.21) increased mesh resolutions parallel to the wall are necessary in order to resolve the small scale structures in the heat flux distribution.
5.4.4.3 Influence of the local velocity and temperature fields

Figure 5.28 shows the instantaneous velocity distributions in the radial, azimuthal and axial directions on a horizontal slice at \( z = -0.1875 \text{ mm} \) together with the heat flux through the cylinder head at 346\(^\circ\)CA. The magnitudes of the two wall-parallel velocity components are significantly higher compared to the axial velocity, as a result of the dampening effect at the wall. The flow structures for \( v_r \) and \( v_\varphi \) appear relatively large and uncorrelated with the local wall heat flux. On the other hand, a clear correlation between \( v_z \) and the heat flux can be observed. Velocities towards the walls (blue) correspond to increased wall heat fluxes (yellow), while axial velocities away from the wall (red) correlate with reduced wall heat fluxes (blue).

In the upper row of figure 5.29 the instantaneous axial velocity is illustrated on horizontal slices at axial positions \( z = -3.75, -0.9375 \) and -0.375 \( \text{mm} \). Depending on the distance from the wall, significant differences in the flow structure can be observed: at \( z = -3.75 \text{ mm} \) (figure 5.29(a)) zones with axial velocities towards the wall (blue) are separated from zones with velocities away from the wall (red). Closer to the wall at \( z = -0.9375 \text{ mm} \) (figure 5.29(b)), the axial velocity shows a more distorted structure and increased spatial velocity gradients. In regions with at \( z = -0.375 \text{ mm} \) an axial velocity towards the wall localized ejection streams with an inverse flow direction can be observed (red areas). Closer to the wall (\( z = -0.375 \text{ mm}, \) figure 5.29(c)) the ejection streams become even more pronounced. They appearance is structured, since they tend to cut regions with a flow towards the wall in the shortest possible distance, which is indicated at
Figure 5.28: Azimuthal, radial and axial velocity on a horizontal slice 0.1875 mm below the cylinder head at 346°CA and the heat flux through the cylinder head at 346°CA.

positions A, B and C in figures 5.29(a) - (c).

The lower row of figure 5.29 shows temperature distributions at the corresponding locations. At $z = -3.75 \text{ mm}$ the temperature is uncorrelated with the axial velocity and the heat flux (figure 5.28(d)). With decreasing wall distance ($z = -0.9375$ and $z = -0.375 \text{ mm}$), smaller structures in the temperature field emerge, which correlate with the axial velocity and heat flux distributions. The flow and temperature distributions in figure 5.29 illustrate the $v'_z T'$ correlation curves shown in figure 5.20, which at 346°CA peak at a wall distance of approximately 0.375 mm, while no correlation is
5.4. Results and discussion

Figure 5.29: Axial velocity and temperature on horizontal slices (a) at $z = -3.75 \text{ mm}$ ($y^* = 180$), (b) $z = -0.9375 \text{ mm}$ ($y^* = 46$) and (c) $z = -0.375 \text{ mm}$ ($y^* = 23$) at $346^\circ \text{CA}$.

found for wall distances larger than 2.7 mm.

The previously described behavior of the axial velocity close to the wall is schematically illustrated in figure 5.30(a). On the left side of the schematic the fluid moves towards the wall. With decreasing wall distance the increased number of ejection streams result in relatively higher and distorted heat fluxes at the wall. On the other hand, in zones where the fluid moves away from the wall relatively low and uniformly heat flux distributions can be observed.

The strength of the ejection streams close to the wall can be quantified by the magnitude of the wall parallel vorticity components $\tau_{wn}$ (figure 5.30(b)). All curves show relatively constant low values in the inner cylin-
der which at a certain distance from the cylinder head increase sharply with decreasing wall distance. The distances where the curves start to increase agree well with the boundary layer thicknesses reported in figure 5.21 at a threshold percentage of 80%. The increasing vorticity magnitude at the wall towards TDC indicates increasing strength of the ejections streams, which is in agreement with figure 5.29. The reduced vorticity at 360°CA can be attributed to the decreased turbulent kinetic energy at TDC (table 5.2).

The transport of colder gas from the boundary layer into the bulk gas due to the wall normal velocity component is responsible for the increased thermal stratification during the compression stroke, which have been observed in several LIF engine studies [36–38, 40]. As indicated in figure 5.30(a) at different wall distances the ejection streams transport cold gases from the boundary layer into the inner cylinder. The largest entrainment of cold gases in the inner cylinder can be observed in regions with a mean flow directed mainly away from the wall. Thus, the development of thermal stratification is mainly influenced by the flow field during compression.

In order to quantify the observed correlations between gas phase and heat flux, figure 5.31 shows scatter plots of temperature at $z = -0.09375$ and -0.375 mm and heat flux at the cylinder head. The x-coordinate of every point represents the temperature at the given wall distance and a radial and azimuthal position $r_1$ and $\varphi_1$. The corresponding value for the y-axis of the same point is the heat flux at the cylinder head with the same radial ($r_1$) and azimuthal ($\varphi_1$) position. The black line is a $4^{th}$ order polynomial
5.4. Results and discussion

Figure 5.30: (a) Schematic of the flow behavior close to the wall; (b) wall horizontal vorticity magnitude versus wall distance.

Regression curve and the correlation coefficient $R^2$ is defined as follows:

$$R^2 = \frac{\sum_{k=0}^{n}(f_i - \bar{y})^2}{\sum_{k=0}^{n}(y_i - \bar{y})^2} \quad (5.7)$$

where $n$ is the number of points in the scatter plot, $f_i$ the regression curve value at point $i$, $\bar{y}$ is the mean heat flux and $y_i$ is the heat flux corresponding to point $i$.

Close to the wall ($z = -0.09375 \ mm$) a stronger correlation between temperature and heat flux can be seen (figure 5.31(a)): higher temperatures are associated with higher heat fluxes. The regression curve decreases almost linearly between 500 $K$ and 950 $K$ and the gradient increases significantly for $T > 950 \ K$. This behavior is related to the correlation between temperature and axial velocity close to the wall (figure 5.20). High temperatures close to the wall are observed at points with velocities directed towards the wall, which additionally increase the local heat flux and ex-
Figure 5.31: Scatter plot of the heat flux and the temperature at (a) $z = -0.09375 \ mm$ and (b) $z = -0.375 \ mm$ at 346°CA.

This explains the increased gradient of the curve for higher temperatures. Farther away from the wall the correlation coefficient is significantly reduced, which at $z = -0.375 \ mm$ results in a $R^2$ value of 0.26 (figure 5.31(b)).

In figure 5.32(a) the correlation coefficients of temperature and heat flux fields are plotted versus the wall distance at several times during the compression stroke. The curves reveal two trends: first, with decreasing wall distance the correlation coefficients of all curves move towards $R^2 = 1$. This is reasonable, since the heat flux is calculated based on the temperature gradients at the wall. Secondly, the decreasing correlation coefficients towards TDC are related to the decreasing boundary layer thickness reported in figure 5.21.

The correlation coefficients of the wall-normal velocity with the heat flux are shown with respect to the distance from the cylinder head in figure 5.32(b). The coefficients increase from $R^2 < 0.2$ at 3.75 $mm$ to maximum values between 0.38 and 0.5 at distances to the cylinder head between 0.08
5.4. Results and discussion

and 0.4 mm. Closer to the wall decreasing R² values are obtained, which are attributed to the zero velocity boundary condition. Similar to figure 5.32(a) a decreasing trend towards TDC can be seen, which is also related to the decreasing boundary layer thickness.

Close to the wall the correlation coefficient of the temperature field is significantly higher compared to the R² values of the wall-normal velocity. Farther away from the wall low correlation coefficients can be observed for both fields.

In figures 5.32(c) and (d) the x-axis is transformed into wall-normal coordinates based on the semi-local scaling, resulting in a collapse of the curves throughout compression. The temperature correlation coefficients in figure 5.32(c) are relatively low in the log-law region (\(y^* > 20\)). With decreasing wall distance (\(y^* < 20\)) the correlation coefficients increase to reach values close to one in the viscous sublayer (\(y^* < 8\)). The maximum R² values in the wall-normal velocity field (figure 5.32(d)) are located at approximately \(y^* = 10\), which corresponds to the peak in the correlation curve between temperature and wall normal velocity \(\langle v' T' \rangle_z^*\) in figure 5.20. For \(y^* > 50\), R² drops to values between 0.15 and 0.2. In general the collapsing curves indicate a constant correlation in wall-normal units between gas phase and heat flux during the whole compression stroke.

The correlation coefficients in figure 5.32 are a good indicator for the resolution requirements at the wall during the compression stroke in ICEs. The nearest cell at the wall must be located within the viscous sublayer (\(y^* < 8\)) in order to accurately predict the local heat flux. In addition the
5. DNS of the Compression Stroke under Engine-like Conditions

Figure 5.32: Correlation coefficient ($R^2$) of temperature (a,c) and axial velocity (b,d) with wall heat flux at different wall distances and piston positions. The wall distances are plotted in dimensional form [mm] (a,b) and in wall-normal units ($y^*$) using semi-local scaling (c,d).

resolution in wall parallel direction must be small enough to resolve the smallest structures shown in figure 5.28.

The heat flux at the cylinder head and the wall-normal velocity distribution at $z = -3.75$ mm are plotted in figure 5.33(a) and (b). In spite of the low correlation coefficient at this time and wall distance ($R^2 < 0.1$) visually a clear correlation between the wall-normal velocity and the heat

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flux can be discerned. As already shown in figure 5.30(a) regions with a flow towards the wall (blue) are associated with an average higher and strongly fluctuating heat flux distribution, while regions with a flow away from the wall have a relatively low and more uniform heat flux distribution. The ejection streams, which are responsible for the high spatial variation of the wall heat flux, can only be observed close to the wall ($y^* < 20$). This explains the relatively low correlation coefficients of the wall-normal velocity field further away from the wall. But as shown in the figures 5.33(a) and (b) the wall-normal velocity can predict the average and the fluctuation level of the local wall heat flux.

Figure 5.33(c) and (d) shows the wall-normal velocity and the heat flux on a coarser mesh with a resolution of 1.5 $mm$ at 346$^\circ$CA. The coarse grid values are derived by averaging the high resolution DNS data within the coarse cells. The resolution of 1.5 $mm$ has been chosen, since it is large enough to filter out small scale spatial fluctuations and small enough to resolve large structures. In addition 1.5 $mm$ is in the range of commonly grid sizes in LES engine calculations [45].

When comparing the wall normal velocity and the heat flux on the coarse mesh, visually a higher correlation of the heat flux and the wall-normal velocity distributions can be seen (figures 5.33(c) and (d)).

In figure 5.34 correlation coefficients at 346$^\circ$CA of the high resolution DNS mesh are compared with the coarse grid at different wall distances. Close to the wall, the influence of local ejection streams is captured by the wall-normal velocity field and thus similar $R^2$ values between the coarse
Figure 5.33: Wall heat flux through cylinder head and wall-normal velocity on a horizontal slice at $z = -3.75$ mm on the DNS grid and on a coarser grid with a resolution of 1.5 mm.
5.4. Results and discussion

grid and the DNS mesh can be observed. With increasing wall distance fewer ejection streams are visible in the velocity field resulting in decreasing correlation coefficients for the DNS mesh. In contrast to this the high fluctuations in the heat flux distribution are averaged out in the coarse mesh following by significant increased correlation coefficients. In contrast to the wall-normal velocity no improvement of the temperature correlation coefficients on the coarser grids can be observed.

5.4.4.4 Joint probability density functions

The correlations between two fields can be described in more detail by using 2D Probability Density Functions (joint PDF). The joint PDF distribution are derived as follows: the heat flux at the cylinder head (plane 2 in figure 5.35) is point-wise correlated with the wall normal velocity or temperature
distribution on the horizontal plane with a distance of $dz$ from the cylinder head (plane 1). Since the mesh is extruded in the axial direction it is possible to compare the value of the grid point at the cylinder head to the grid point on plane 1 with identical radial and azimuthal coordinates. The scatter plots shown in figure 5.31 illustrate the discrete heat flux (y-axis) and temperature (x-axis) values for all nodes on the horizontal slides.

The derivation of the 2D PDF expresses the probability of a certain combination of velocity/temperature and wall heat flux and plot in a contour plot. Red areas indicate a high probability of heat flux and wall normal velocity pairs, while white areas are connected to a nearly zero probability.

The joint PDFs of the wall normal velocity with the heat flux at two times ($306^\circ$ and $346^\circ$CA) and at two wall distances (0.375 and 0.9375
mm) are shown in figure 5.36. Towards TDC the global heat transfer increases significantly resulting in stretching of the joint PDFs with increasing time. Thus, the heat flux values reported in figures 5.37 and 5.38 are non-dimensionalized by the average heat flux on the cylinder head. With increasing wall distance the wall normal velocity magnitude increases resulting in a wider spread of the joint PDF distributions in figure 5.36. For relative comparisons with different wall distances the x-axis in figures 5.37 and 5.38 is non-dimensionalized by the averaged wall normal velocity magnitude at the selected wall distance. The temperature is always non-dimensionalized by the constant wall temperature of 500 [K].

Figure 5.37 shows the joint PDFs of the temperature and wall normal velocity with the heat flux at 346°CA for four different wall distances. The joint PDFs of the heat flux with temperature (figure 5.37(a)) reflects the decreasing correlation coefficients with increasing wall distance (shown in figure 5.32). At z = -0.1875 mm a clear correlation between the two variables can be seen, which weakens with increasing distance from the wall. At z = -0.9375 and z = -3.75 mm the shape of the joint PDF is nearly one-dimensional and temperature and heat flux become uncorrelated.

Compared to the temperature field the joint PDF of the wall-normal velocity (figure 5.37(b)) shows a weaker correlation with the heat flux at z = -0.1875 mm, as indicated by the broader PDF shape. With increasing wall distance the joint PDF transforms from an almost linear shape at z = -0.1875 mm to a triangular shape at z = -0.375 mm. This can be seen by comparing gradients of the marked curves in figure 5.37(b). The gradients
of curves A1 - A4 remain unaffected, while curves B1 - B4 are rotated until B4 is almost vertical. The rotation of curves B1 - B4 is due to the ejection streams close to the wall (figure 5.30), which are only created if the fluid moves towards the wall (positive $v_z$). At $z = -0.1875 \text{ mm}$ the ejection streams are captured by the axial velocity and the joint PDF has an almost linear shape. With increasing distance from the wall fewer ejection streams can be observed, which results in an increasing gradient from B1 to B4. The slopes of curves A1 - A4 remain constant, since for $v_z < 0$ (flow away from the cylinder head) no ejection streams are formed. A similar behavior can be seen at all observed times during compression.

Figure 5.36: Dimensional joint PDFs of the heat flux and the wall normal velocity at 306°CA and 346°CA at different wall distances.
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Figure 5.37: (a) Joint PDF of temperature vs. heat flux at 346°CA; (b) Joint PDF of the wall-normal velocity vs. the heat flux at 346°CA.

At a constant wall distance of $y^* = 9.2$ the joint PDFs at several times during compression collapse (figure 5.38), indicating a constant correlation in wall-normal units between wall-normal velocity and heat flux during the whole compression stroke. Thus, for the investigated setup the influence of wall-normal velocity on local wall heat flux can be predicted based on the joint PDF as a function of $y^*$. This can possibly be used as a base for the development of novel engine wall heat transfer models in 3D CFD calculations. In case the mesh resolution in RANS or LES calculations is too coarse to capture the small structures of the wall heat flux, the joint PDFs reported figure 5.37 can be used to statistically describe the heat flux.
5. DNS of the compression stroke under engine-like conditions

\[ y^* = 9.2 \]

\begin{align*}
\text{225°CA} & \quad \text{270°CA} & \quad \text{306°CA} \\
\text{333°CA} & \quad \text{346°CA} & \quad \text{360°CA}
\end{align*}

Figure 5.38: Non-dimensional joint PDFs at different piston positions with a wall distance of \( y^* = 9.2 \).

distribution within a coarse cell.

5.4.5 Influence of the thermal conditions at BDC

Numerical simulations offer the advantage that initial and boundary conditions can be freely chosen, which allows for isolating processes in order to assess their effects. In this section the effects of the initial temperature distribution at BDC on temperature and heat transfer evolution during compression are evaluated by initializing the thermal field at BDC with a uniform temperature equal to the average temperature of the thermally stratified case. The boundary conditions and the piston movement are in
both cases identical to the compression setup described in section 5.2. In both simulations the identical velocity field described in section 5.3 is initialized and the composition is a uniform unburnt $\lambda = 2 \, \text{H}_2/\text{air}$ mixture.

The temperature distributions on vertical slices of the uniform case (upper row) and the stratified initial temperature case (lower row) are shown in figure 5.39. At $181^\circ\text{CA}$ the reduced temperatures at the walls in the uniform case are due to heat losses. Already at $225^\circ\text{CA}$ the differences between both cases are strongly reduced, and the main difference is the higher temperature close to the cylinder head in the stratified case, resulting from the entrained hot gases in the core of the vortex ring (figure 5.2). At $270^\circ\text{CA}$ the region close to the cylinder head also shows a good agreement between the two cases.

The temperature PDFs in the whole cylinder plotted in figure 5.40 show that at $225^\circ\text{CA}$ the distributions only differ in their peak values.

At $270^\circ$, $306^\circ$ and $333^\circ\text{CA}$ the temperature PDFs for both cases are nearly identical. Close to TDC at $346^\circ\text{CA}$ again a small deviation in the peak value can be observed, which is attributed to the high sensitivity of the heat transfer on small differences in the flow field close to TDC.

A comparison of the global wall heat losses is shown in figure 5.41. The heat losses are computed at six time instants during compression, indicated by the circles and the curves are cubic interpolation splines. Up to $333^\circ\text{CA}$ heat losses between the homogeneous and the stratified case are nearly identical, while at $346^\circ\text{CA}$ the heat loss in the stratified initialization is slightly lower. The deviations in the wall heat losses close to TDC are
related to the coupling of temperature and flow field due to density. The homogeneous temperature at BDC imposes a small deviation in the flow field, which has only a minor influence on the global wall heat transfer until 333°CA. Close to TDC the heat losses are very sensitive to small differences in the flow field, since at this time the temperature gradients at the walls reach their maximum.

The influence of the thermal situation at BDC is found to be practically negligible for the setup and conditions considered here. The evolution of temperature and wall heat transfer during compression is mainly influenced
5.4. Results and discussion

Figure 5.40: (a,b) Probability density functions of the temperature of stratified and homogeneous initialization at several piston positions during compression.

Figure 5.41: Comparison of the heat losses between stratified and homogeneous initialization during the compression.
by the wall temperature and the flow field at BDC. This finding can explain why the use of different intake air temperatures for each port in Kakuho et al. [141] and Herold et al. [142] had only limited success in increasing thermal stratification at TDC of the compression stroke.

5.5 Summary and conclusions

In this chapter the compression stroke which takes into account the fully resolved velocity and thermal boundary layer under engine relevant conditions is investigated using DNS. The initial conditions are derived from a separate DNS of the intake stroke involving thermal and composition mixing, avoiding the use of artificial initial and boundary conditions. Comparisons with mesh resolutions typically employed in the literature and with the Kolmogorov scale showed sufficient mesh resolution at the walls and inside the cylinder.

During the compression stroke significant changes in the flow field and thermodynamic properties are observed. Until approximately 270°CA, the mean flow field is dominated by the central vortex ring. At later times the vortex ring disintegrates and the mean flow is mainly defined by the axial velocity imposed by the piston motion. With decreasing piston speed towards TDC the turbulent kinetic energy increases significantly compared to the kinetic energy of the mean flow. The strongly increasing pressure plays a dominant role since it results in strongly decreasing kinematic viscosities, reduced turbulent length scales and strongly increased dissipation rates towards TDC.
The average temperature increases due to compression from approximately 540 $K$ at BDC to around 1100 $K$ at TDC. Temperature fluctuations also increase significantly towards TDC, which in case of HCCI and related combustion modes will have a strong impact on the burning duration and autoignition timing. Responsible for the increased temperature fluctuations is the wall normal velocity component, which locally transports cold gases from the boundary layer into the bulk gas. In contrast to the temperature field, the species distribution becomes almost uniform at TDC. Thus, for the considered setup and conditions, hot combustion products remaining from the previous cycle have very small impact on the temperature stratification close to TDC. These findings agree with the experimental observations reported in [37, 40, 129].

The focus of this chapter lies on the investigation of the velocity and thermal boundary layers and heat transfer during compression. The rapidly increasing heat flux towards TDC is mainly attributed to the decreasing kinematic viscosity, which is followed by increasing temperature and velocity gradients at the walls. This results in decreasing boundary layer thicknesses and decreasing size of the heat flux structures towards TDC. Thus wall-resolved LES require, in addition to refinements in the wall normal direction, higher grid resolutions in the wall parallel directions as well.

In wall-normal units, collapsing profiles of the velocity and thermal boundary layer in the viscous sublayer ($y^+ < 8$) can be observed during the compression stroke. By using the semi-local scaling, which also takes the influence of the local density variations into account, the curves collapse...
also in the buffer and the outer layer regions \((y^* > 8)\). The same collapsing behavior can be observed at all engine walls. In agreement with the experiment \([2]\), no logarithmic profile was found. This can be attributed to the time varying geometry and the changes it imposes on the global flow field compared to channel or pipe flows. This finding indicates that the commonly used wall function approach, which is based on the law-of-the-wall needs to be re-considered for the development of novel wall models for engine flows.

Close to the wall \((y^* < 8)\), the temperature field correlates strongly with the wall heat flux \((R^2\) value close to 1). With increasing wall distance the correlation weakens and for \(y^* > 20\) temperature and heat flux become nearly uncorrelated. The wall-normal velocity on the other hand remains correlated with the heat flux at the wall at large distances from the wall. A flow towards the wall results in a strongly varying and higher heat flux, which is due to local ejection streams close to the walls. In regions with a flow away from the walls, relatively uniform and low heat fluxes are observed. The relatively low correlation coefficients between wall-normal velocity and heat flux are attributed to the distortion of the heat flux distribution by the ejections close to the walls \((y^* < 30)\). In case the influence of these ejections is filtered out by averaging on coarser grids, farther away from the wall strongly increased correlation coefficients can be observed.

In summary, farther away from the wall the wall-normal velocity is responsible for the convective transport of hot/cold gases towards/away from the wall. This determines the temperature distribution close to the walls.
and thereby the local heat flux distribution. The behavior is quantified by the correlation between temperature and wall-normal velocity fluctuations, which peak at approximately $y^* = 20$.

The joint PDFs of the heat flux with the wall normal velocity show that for constant non-dimensional wall distances an almost identical correlation between wall-normal velocity and heat flux can be observed during the whole compression stroke. If this also applies to higher turning speeds and more complex geometries it can be used to statistically describe the heat flux distribution within the coarser cells used in LES or RANS calculations. Thus it can improve existing wall models or serve as a starting point for future engine wall models.

The effect of the initial temperature distribution on the PDF of temperature and wall heat losses was also investigated by considering a uniform initial temperature in the cylinder. It was found that the heat losses and the temperature field evolution during compression are mainly defined by the flow field at BDC and the wall temperature and the thermal initial conditions play only a minor role. This implies that increasing thermal stratification cannot be achieved by perturbing the temperature field at BDC (e.g. with different temperature levels in the two intake channels as tried in Krasselt et al. [143] and Herold et al. [144]). More efficient in this regard would be modifications of large flow structures and variations of the wall temperatures.
Chapter 6

Conclusions and outlook

To the best of our knowledge for the first time accurate numerical experiments on a laboratory-scale engine-like setup were performed, which has also been studied experimentally [1]. The spectral element method employed in the DNS allowed for the accurate description of the complex geometry which consisted of a fixed open valve, a moving piston and a large plenum upstream of the valve. The geometric arrangement ensures an accurate description of the flow within the valve and at the inflow to the cylinder and eliminates the need of using artificial initial and boundary conditions. The incompressible DNS was validated against the experimental data of Morse et al. [1] showing very good agreement with respect to mean and rms velocity profiles at all measured times and locations.

Despite identical boundary conditions, significant CCVs in the flow field were observed in the multiple-cycle flow calculation consisting of 11 consecutive cycles. The investigation of the basic cause-and-effect relationships show strong coupling between consecutive cycles. During the intake
6. Conclusions and outlook

stroke a hollow jet flow enters into the cylinder, whose trajectory is strongly
influenced by the radial velocity remaining at TDC of the previous cycle.
Towards the end of the intake stroke the jet forms a large central vortex
ring, which is influenced by the nozzle geometry and the engine walls. The
strength and stability of this vortex ring depends sensitively on the jet tra-
jectory and has in turn a strong effect on the flow field at TDC of the
subsequent cycle.

The observed CCVs of the flow field can be only applied to engine types
with a central intake valve configuration. In case of tumbling or swirling
intake configurations differences in the CCV behavior are expected, but
some of the observed couplings (e.g. the interaction between in-cylinder
flow field and jet trajectory) may also be relevant for these engine config-
urations. Furthermore, the data can be used to assess which LES models
and mesh resolutions are capable of capturing the CCVs in this flow field.
The time and location of possible deviations can be identified, which allows
to effectively improve LES turbulence models in ICEs.

The second part of this work investigates the effect of the compres-
sion stroke on the flow, temperature and species fields under engine relevant con-
ditions. For the compressible calculations the valve is closed at BDC and
the initial conditions are taken from a separate DNS of the intake stroke
involving thermal and composition mixing. The analysis aims firstly at iden-
tifying the relevant processes affecting wall heat transfer. It was found that
the decrease of the kinematic viscosity resulting from the increasing pres-
sure has a strong effect on the flow leading to significant smaller turbulent
length scales. This result in increasing temperature gradients at the walls, which is followed by heat fluxes which increase beyond what one would expect only from the increasing cylinder temperatures due to compression.

The strong local correlation of the temperature with the heat flux to the walls in regions close to the wall \((y^+ < 8)\) weakens with increasing distance from the walls. On the other hand, the wall-normal velocity remains strongly correlated with the local heat flux even far away from the walls. A local flow directed away from the walls results in relatively low and uniform heat fluxes, while local velocities towards the walls are followed by strongly varying and on average higher heat fluxes. The strong fluctuations are found to be attributed to ejection streams in the flow field close to the walls.

Wall heat transfer in CFD engine simulations is mainly modeled using wall functions, which are based on the law-of-the-wall. In agreement with experiments [2], no logarithmic profile was found in this work, which has to be considered for the development of novel CFD engine wall heat transfer models. When transforming the wall distance into density-weighted wall-normal units a collapse of the velocity and thermal boundary layers to essentially one profile during the whole compression stroke can be observed. Furthermore, for constant wall distances in wall normal units, the correlation between wall-normal velocity and heat flux is shown to be nearly identical during the whole compression stroke. If these findings apply also for higher turning speeds and tumbling or swirling intake configurations they can be used to extend existing ICE wall heat transfer models or serve
6. Conclusions and outlook

as a starting point for the development of novel engine wall models.

The effect of the initial conditions for temperature was investigated by repeating the simulation of the compression stroke starting with a uniform temperature field inside the cylinder. It is found that the temperature initial conditions are quickly forgotten and that the spatio-temporal evolution of the temperature field and heat transfer during compression is almost fully determined by the flow field at BDC and the wall temperature. Thus for the investigated conditions the effect of the temperature distribution at BDC is practically negligible.

The results provide unique insights into the variation of the flow, temperature and composition fields in the investigated engine-like geometry, with a high temporal and spatial resolution that cannot be achieved even by sophisticated experiments. Up to now the parameter values in currently available RANS and LES turbulence models used in ICE simulations have been obtained using data from simple setups (e.g. homogeneous turbulence simulations in periodic cubic domains [15]), which differ substantially from the flow in engine geometries featuring interaction of intake-created shear flows with walls and subsequent compression. Although the geometry employed in this work is simplified, the flow field contains many of the important flow features of ICEs. Thus, one of the main contributions of this work is to provide a validation platform of ICE turbulence and wall heat transfer models, which in such spatiotemporal-resolution are not obtainable by experimental methods.

While only one compression cycle is investigated in this work, ongoing
simulations of the compression stroke using the flow fields from different cycles of the multi-cycle simulation show that although large flow structures have an influence on the flow and temperature field, the observed trends are very similar for all calculated cycles.

The investigated valve-piston assembly has been carefully chosen as a first step towards DNS of real engines with higher geometric complexity and more realistic conditions. For future work, one should investigate if the findings from this work also apply to higher rotational speeds and more complex geometries inducing tumbling or swirling motions as well as bowl-in-piston geometries that induce a squish flow around TDC. Of special interest would be a comparison between DNS and experimental high-speed PIV/LIF measurements. Direct numerical simulations are hindered by the high computational cost, which restricts the maximum rotational speed and the number of simulated cycles. Optical PIV and LIF measurements in ICEs provide very useful insights in real engine setups but are limited by the access into the cylinder and the restricted spatial and temporal resolution. Appropriately designed experiments which are accessible by DNS will compensate for the weaknesses of each approach to provide much deeper insights for engine design and development.

Furthermore, the fields at TDC are excellent initial conditions for reactive simulations, since they avoid the use of the commonly used artificial turbulence. Of special interest would be the investigation of the auto-ignition behavior under HCCI relevant conditions and the interaction of the early flame kernel with the complex flow and temperature fields.
A.1 Assessment of the averaging approach

A combination of azimuthal and ensemble averaging was used to obtain converged statistics. The number of statistically independent points in the azimuthal direction can be estimated based on the maximum influencing length of two fluid particles (estimated by two point correlations) and the circumference. At 90°CA and for $r/R_c > 0.3$, the number of independent averaging points is at least 85 for a combination of azimuthal and ensemble (i.e. total) averaging over six cycles. The azimuthal velocity $v_\phi$ is a good indicator to evaluate statistical convergence, since, because of axis-symmetry, the average value should be close to zero. Figure A.1 shows the instantaneous, the spatially averaged value for cycle 3 and the spatial and ensemble averaged $v_\phi$ at 22.5 $mm$ below the cylinder head and 90°CA. Time and location have been chosen in the area of the highest mean and rms velocities in the flow field. The instantaneous value (solid line) fluctuates between -2 and 2 $m/s$. With spatial averaging (dash-dotted curve), the values for
$r/R_c \gtrsim 0.5$ are close to zero. With azimuthal and ensemble averaging, converged statistics are obtained already for $r/R_c \gtrsim 0.3$. Close to the cylinder axis the number of samples is too small to obtain converged statistics.

![Figure A.1](image.png)

Figure A.1: Instantaneous (solid line), azimuthal (dot-dashed line), and total average (dashed line) azimuthal velocity at $z = -22.5 \text{ mm}$ at $90^\circ$CA.


Bibliography


Curriculum Vitae

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