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Numerical Simulations of Spray A Split Injection using LES-CMC

Master Thesis

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Abstract

Numerical simulations are performed for an n-dodecane spray flame (Spray A split injection from Engine Combustion Network) using the Conditional Moment Closure (CMC) model coupled with Large Eddy Simulation (LES). A 54-species skeletal mechanism was used to represent the chemistry. Engine-relevant configurations are investigated, namely a diesel-like and a low temperature combustion-like (LTC) condition. The comparison of the experimental and simulated non-reactive vapour penetration length shows that both injection lengths are correctly predicted and therefore also the slipstream effect of the first injection. A CMC grid sensitivity analysis for the first injection under the diesel-like condition shows how one 1D and two 2D-CMC grids (a coarse and a fine type) produce significantly different flame structures and ignition processes. The result is that the radial transport of conditional moments is necessary to achieve a realistic flame structure around the lift-off length. A two-dimensional CMC discretization is therefore required for the simulation of a transient, non-premixed flame. Assessment of the combustion process shows that the most realistic and detailed predictions are achieved by the fine resolution. The computational cost of the fine 2D-CMC grid is a factor of two compared to the 1D type and is the recommended option. The full split injection for both the diesel and the LTC-like condition is simulated using LES-CMC. The ignition delay time is captured accurately for the former (+0.6 %) and slightly too early for the latter (−9 %) case. An ensemble average of the diesel-like case of total 5 realizations and a single realization for the LTC-like condition is compared to the experiment. The qualitative prediction of formaldehyde and soot precursor production and consumption in time and space is accurate, however the evaluation of the lift-off length remains inaccurate. The pressure rise is seen lower than the experimental measurement, whereas a further test using the direct integration combustion model shows better trends. The simulation of the LTC-like case indicated that the main ignition event is initiated by the second injection leading to ultra-low soot emissions.
# Nomenclature

## Symbols

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
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</thead>
<tbody>
<tr>
<td>$D$</td>
<td>Molecular Diffusivity</td>
</tr>
<tr>
<td>$e$</td>
<td>Internal energy</td>
</tr>
<tr>
<td>$G$</td>
<td>Filter function, related to LES</td>
</tr>
<tr>
<td>$h$</td>
<td>Enthalpy</td>
</tr>
<tr>
<td>$k_r$</td>
<td>Residual turbulent kinetic energy</td>
</tr>
<tr>
<td>$m$</td>
<td>mass</td>
</tr>
<tr>
<td>$N$</td>
<td>Number of reactants</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure</td>
</tr>
<tr>
<td>$\overline{P}(\eta)$</td>
<td>Density-weighted filtered PDF</td>
</tr>
<tr>
<td>$Q_a$</td>
<td>Conditionally filtered species</td>
</tr>
<tr>
<td>$Q_h$</td>
<td>Conditionally filtered enthalpy</td>
</tr>
<tr>
<td>$R_u$</td>
<td>Universal gas constant</td>
</tr>
<tr>
<td>$S_{ij}$</td>
<td>Rate-of-strain tensor</td>
</tr>
<tr>
<td>$S_c$</td>
<td>Schmidt number</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
</tr>
<tr>
<td>$u_i$</td>
<td>Components of velocity vector, $i=(1,2,3)$</td>
</tr>
<tr>
<td>$\overline{W}_\eta$</td>
<td>Mean molar mass</td>
</tr>
<tr>
<td>$X$</td>
<td>Mole fraction</td>
</tr>
<tr>
<td>$[X_a]$</td>
<td>Species $a$</td>
</tr>
<tr>
<td>$Y$</td>
<td>Mass fraction</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Correlated to $\beta$-PDF parametrization</td>
</tr>
<tr>
<td>$\Delta$</td>
<td>Filter width</td>
</tr>
<tr>
<td>$\epsilon_r$</td>
<td>Sub-grid scale or residual dissipation</td>
</tr>
<tr>
<td>$\eta$</td>
<td>Sample space variable of mixture fraction $\xi$</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic viscosity</td>
</tr>
<tr>
<td>$v$</td>
<td>Kinematic viscosity</td>
</tr>
<tr>
<td>$\tilde{\xi}$</td>
<td>Resolved mixture fraction</td>
</tr>
<tr>
<td>$\bar{\xi}^{\tilde{\xi}/2}$</td>
<td>Sub-grid scale variance of the mixture fraction</td>
</tr>
<tr>
<td>$\rho$</td>
<td>Density</td>
</tr>
<tr>
<td>$\tau_{ij}^R$</td>
<td>Residual or sub-grid scale stress tensor</td>
</tr>
<tr>
<td>$\tau_{ID}$</td>
<td>Ignition delay timing</td>
</tr>
<tr>
<td>$\chi$</td>
<td>Scalar dissipation rate</td>
</tr>
<tr>
<td>$\omega$</td>
<td>Chemical source term, rate of consumption or production</td>
</tr>
<tr>
<td>$(.)</td>
<td>\eta$</td>
</tr>
</tbody>
</table>
Subscript Indices

\( \alpha \) Species index
\( d \) Related to droplets
\( \eta \) Conditioned on \( \xi = \eta \)
\( r/sgs \) residual or sub-grid scale, related to filtering operation
\( st \) At stoichiometric conditions
\( t \) Relating to turbulence

Acronyms and Abbreviations

AHRR Apparent Heat Release Rate
ASOI After Start of Injection
Case 1 Diesel-like condition (900 K ambient gas temperature)
Case 2 LTC-like condition (750 K ambient gas temperature)
\( \text{CH}_2\text{O} \) Formaldehyde, low-temperature combustion indicator
\( \text{C}_2\text{H}_2 \) Acetylene, specie that leads to soot formation
CMC Conditional Moment Closure
CFD Computational Fluid Dynamics
DI Direct Integration
DNS Direct Numerical Simulation
ECN Engine Combustion Network
ETHZ Eidgenössische Technische Hochschule Zürich
HCCI Homogeneous Charge Compression Ignition
ID Ignition Delay
KHRT Kelvin-Helmholtz & Rayleigh-Taylor droplet break-up model
LES Large Eddy Simulation
LTC Low Temperature Combustion
MFT Total mixture fraction
MF1/MF2 Mixture fraction one / two
\( n \)-dodecane Fuel \( \text{C}_{12}\text{H}_{26} \), diesel surrogate
\( \text{NO}_x \) A generic term for NO (nitric oxide) and NO2 (nitrogen dioxide)
OH Hydroxide, a radical specie formed at the flame front
PAH Polycyclic Aromatic Hydrocarbons
PCCI Premixed Charge Compression Ignition
(F)PDF (Filtered) Probability Density Function
PLIF Planar Laser Induced Fluorescence
RANS Reynolds Averaged Navier-Stokes
R-D Reitz-Diwakar atomization model
Re Reynolds Number
Chapter 1

Introduction

The internal combustion engine was invented more than a hundred years ago (e.g. the Diesel engine, 1893) and has been prevailing as the dominant powertrain for cars, motorcycles, trucks, ships, agriculture and construction machinery ever since. The simple reason why it has not been displaced is that the large power density of fossil fuels is not yet reached by batteries and fuel cells. Moreover, recharging the vehicle by means of fuel in liquid form is the most efficient, fastest and most convenient way, rather than charging the battery for several hours or refuelling a high pressure, liquid hydrogen tank. However, there has been considerable effort in increasing the capacity of lithium-ion batteries or in accelerating the charging process of such a device (i.e. charging more than half of the battery-capacity within 30 minutes [35]), which might become a competitive alternative for internal combustion engines.

Nevertheless, more than 750 million passenger cars are used today [51], more than 70 million cars were produced only in 2014 [1], most of them using internal combustion engines, hence society will continue to rely heavily on this type of engine in the foreseeable future. Unfortunately, engine emissions produced by the combustion of fossil fuels entail pollution of the environment whose consequences are critical and have forced governments to tighten pollutant laws. The design and development of clean and efficient internal combustion engines is necessary to meet the stringent regulations concerning pollutant emission and fuel efficiency. The compression ignited engine has a high thermal efficiency and therefore a lower fuel consumption (i.e. also lower CO$_2$ emissions) compared to its counterpart, the gasoline spark ignited engine. However, diesel engines typically have

![Emission map of different combustion principles](image-url)

Figure 1.1: Emission map of different combustion principles [56]
higher NO\textsubscript{x} and soot emissions than gasoline engines, therefore focus has been laid on developing advanced concepts where the advantages of both are blended into one single engine technology. One promising approach to reduce the in-cylinder emissions is to lower the combustion temperature, which is termed as low temperature combustion (LTC). Homogeneous charge compression ignition (HCCI) belongs to the family of LTC and has received increased attention. In HCCI, lean fuel-air-mixture conditions are maintained in the cylinder and ultra-low emissions in connection with high efficiency are possible. An overview over the different types of combustion is visible in figure 1.1.

Increased complexity is however met, since the initiation of combustion is difficult to control. Since state-of-the-art experiments can only provide partial insight into the in-cylinder process due to limited measurement techniques, computational fluid dynamics (CFD) has become an indispensable complement in engine development. One measure to improve engine performance is the use of multiple fuel injections. It has been shown that with multiple injections both soot and NO\textsubscript{x} emissions can be reduced significantly in contrast to the conventional single-pulse injections, where a soot/NO\textsubscript{x} trade-off is met [25]. Increasing the degree of freedom by using two or more injections makes the combustion process less predictable, which makes the role of simulation aiding the design process more important. The use of numerical methods which correctly capture the ignition events of multiple fuel injections becomes essential. The validity of such models has to be confirmed by the direct comparison to recent experimental work. The Engine Combustion Network has characterized a well-known injector with in combination with a constant volume combustion chamber called "Spray A", where \textit{n}-dodecane serves as the diesel surrogate. Skeen et al. [55] used the Spray A setup for a split injection schedule (0.5 ms/0.5 ms dwell/0.5 ms) for a multiple injection experiment. This report focuses on reproducing the experimental findings of [55] by means of LES-CMC, where two operating conditions have been considered, one with 900 K ambient gas temperature as the diesel-like (referred to as "Case 1") and the other with 750 K ambient temperature as the LTC-like (referred to as "Case 2") condition.

The experiment of a Spray A split injection was thoroughly analysed and presented in [55], describing many complex aspects which need to be accounted for while reproducing such a scenario by means of CFD. One difficulty is that the injection pulses are of very short duration (0.5 ms), so neither the flow field of the fuel spray nor the combustion process reach steady state and have therefore a highly transient nature. Another challenge is to correctly address the complex interaction of the first and second injection and their subsequent mixing with the oxidizer. Lastly, for Case 1 it remains to achieve correct prediction of the two individual combustion processes of each fuel spray, where it appears to be noteworthy that the first injection enters a quiescent ambient gas, whereas the second injection meets a highly turbulent flow field with high temperature zones. For Case 2, the situation is different. The lowered bulk temperature leads to only one ignition event after the two sprays have mixed. Therefore, a detailed description of the fluid dynamics as well as the combustion model becomes essential.

Deeper insight into mixing phenomena can be gained by means of large eddy simulation (LES), which is a turbulence model. It has the superior ability to predict details of turbulent mixing and combustion, and its interaction. Despite its finer spatial resolution compared to RANS, the combustion process still takes place on a scale which cannot be resolved by the grid [23]. Therefore, a turbulent combustion model has to be applied for the sub-grid scales.

Non-premixed combustion in the context of RANS using detailed chemical kinetics has successfully been modelled by Conditional Moment Closure (CMC), e.g. [6, 21, 60]. Recently, considerable effort has been dedicated to LES-CMC and has been derived in [39] and further analysed in [57]. Furthermore, it was applied in premixed combustion such as bluff-body stabilized flame [36], partially premixed jet [37], different cases of lifted flames [38], Sandia Flame F [22] and piloted jet flames [23]. LES-CMC of a single \textit{n}-heptane spray has been investigated in [7], where 1D-CMC was applied. The CMC model is a presumed PDF method, in which all the variables are conditioned on the mixture fraction since it is a conserved scalar. The mixture fraction can be described as the
degree of mixing between fuel and oxidizer. The numerical layout of the simulation is as follows: 1) LES equations are resolved on a fine CFD grid on which the momentum equations of the flow are solved, 2) the combustion reactions are resolved on an additional coarser grid on which the CMC equations are solved. The two grids are superimposed, where the CMC-grid is much coarser than the CFD-grid, since the spatial fluctuations of the conditional moments (i.e. reactants and temperature) are much smaller than their corresponding unconditional (i.e. velocity components) ones. This lowers the computational costs of CMC in comparison to direct integration (i.e. computation of chemical reactions in every CFD cell separately) and makes CMC the method of choice for this work. However, this will be investigated later in chapter 5.

The \(n\)-dodecane skeletal reaction mechanism of Yao et al. [62] has been applied which was specifically developed for Spray A simulations. It covers low temperature reactions which are of major importance for Case 2. The chemical mechanism includes 54 species and 269 reactions.

1.1 Report Layout

This report has the following layout. Firstly, the non-reactive vapour penetration length is calibrated in LES. As a next step, also chemical reactions are taken into account and a CMC grid sensitivity analysis is carried out. Three different types of CMC discretizations were tested: one 1D-CMC grid in which the variation of the conditional moments in radial and circumferential direction is neglected and the grid is only refined in the axial direction of the nozzle. The other two types consider 2D-CMC grids with both radial and axial refinement, where a coarse and a fine discretization has been chosen (i.e. one grid has more CMC nodes than the other). It is important to mention that no results from this analysis were compared to the experiment, since multiple simulations for statistics would have been necessary, which is very expensive in terms of computational power and were not run for each CMC refinement. Instead the sensitivity analysis was carried out to investigate a) how much does refinement improve flame structure predictions, b) what is the advantage-to-cost ratio between the different refinements and c) the importance of radial transport of the conditional moments. Point c) was also investigated in [38] and [37] to show that the introduction of radial CMC-transport can generate an improved transition from unburned to burned mixtures near the flame lift-off region. Since the mentioned papers consider steady-state partially premixed jets and flames under low pressure rather than high injection pressure sprays under transient conditions, these findings were verified again.

The last part of this report shows the results and discussion of the full Spray A split injection simulation for both diesel-like and LTC-like operating conditions. Initially the most suitable setup is chosen based on the CMC grid sensitivity analysis. For Case 1, five realizations with identical initial conditions are simulated for ensemble averaging, whereas for Case 2 only one realization was considered. As an additional measure, the setup of Case 1 is simulated by means of the direct integration combustion model to compare the flame structure, pressure rise and cost advantages with LES-CMC. Unless stated otherwise, LES-CMC simulations are considered.

1.2 Aims

This report aims to gain lacking knowledge concerning detailed modelling of multiple diesel injections by means of LES-CMC simulations. The possible findings in this work can be very encouraging and promise deeper insight into advanced, high-tech combustion methods which provide a solid basis for future research. Detailed understanding of this highly transient multiple injections setup and analysis of the mixing state as well as the reaction progress of each injection and the interaction with one another will direct new ways of cleaner, more efficient internal combustion engines.
1.2. Aims
Chapter 2
Methodology

Computational fluid dynamics (CFD) is the analysis of systems involving fluid flow, heat transfer and chemical reactions by means of computer-based simulations. Recently, this method has been gaining strong influence in the design and development of internal combustion engines [58]. In the CFD approach, fluid flows are treated as a continuum and the information of single molecules or atoms is not taken into account. In the following chapter, the general mathematical concepts are presented to describe such a fluid flow. Therefore, a set of governing equations has to be introduced, such as the conservation of mass, momentum and energy. Solutions to such stiff differential equations are obtained means of numerical methods and computational algorithms.

2.1 Basis Conservation Equations

2.1.1 Conservation of Mass

Since matter is neither created nor destroyed in a chemical or fluid system, the condition $dm/dt = 0$ and the conservation over an arbitrary control volume holds

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

(2.1)

where the Einstein Summation Convention has been used. Equation of (2.1) is the conservation equation for total mass and is commonly known as the continuity equation [34].

2.1.2 Conservation of Species

The bulk, mass-weighted velocity $u_i$ results out of the individual velocities $u_{\alpha,i}$ of the various species. In a system of N species, the following definition holds:

$$\sum_{\alpha=1}^{N} \rho_{\alpha} u_{\alpha,i} = \rho u_i$$

(2.2)

Therefore, the difference between $u_{\alpha,i}$ and $u_i$ is the molecular diffusion velocity

$$U_{\alpha,i} = u_{\alpha,i} - u_i$$

(2.3)

Furthermore, the species mass fraction reads $Y_{\alpha} = m_{\alpha}/m$ were $\sum Y_{\alpha} = 1$. The following equation concerns the conservation of $m_{\alpha}$ of the $\alpha$-th species, where two sources can lead to a change. The first is because of chemical reactions and is denoted as $\dot{\omega}_\alpha$ ( mole/(cm$^3$ sec) ) which is of volumetric nature. The second source is a diffusion process over the control surface due to non-uniform concentration. The term $\rho_{\alpha} U_{\alpha,i}$ is the diffusive transport, therefore. Now, the species
conservation equation can be introduced as [34]
\[
\frac{\partial (\rho Y_\alpha)}{\partial t} + \frac{\partial}{\partial x_j} \left[ \rho (u_j + U_{\alpha,j}) Y_\alpha \right] = \dot{\omega}_\alpha
\] (2.4)

**Fick’s Law of Mass Diffusion**

According to [34], a relation for the diffusion velocity can be derived. In the absence of pressure gradient, body force, and thermal diffusion, it can be shown that the diffusion velocity behaves as
\[
U_{\alpha,i} = -D \frac{\partial}{\partial x_i} (\ln Y_\alpha)
\] (2.5)

where it is assumed that the diffusion coefficients of the species are all equal to \(D\) and constant. Equation (2.5) is known as the Fick’s law of mass diffusion.

**Species Reaction Rate**

The species reaction rate is computed according to the basic laws of chemical kinetics which can be found in [34]. It can be derived in the following way [63]. An elemental reaction is considered as:
\[
\sum_{a=1}^{N} v'_{a,j} X_a \rightleftharpoons \sum_{a=1}^{N} v''_{a,j} X_a \quad j = 1, \ldots, N
\] (2.6)

where \(v'_{a,j}, v''_{a,j}\) denote the stoichiometric coefficients of species \(\alpha\) in reaction \(j\) in the forward and reverse direction, respectively, and \(X_a\) is the symbol of species \(\alpha\). The rate of reaction of \(j\) is then
\[
r_j = k_f \prod_{a=1}^{N} [X_a]^{v'_{a,j}} - k_r \prod_{a=1}^{N} [X_a]^{v''_{a,j}} \quad j = 1, \ldots, N
\] (2.7)

The rate of consumption or production of species \(\alpha\) in reaction \(j\) then reads:
\[
\dot{\omega}_{\alpha,j} = (v''_{a,j} - v'_{a,j}) r_j = \frac{d[X_a]}{dt}
\] (2.8)

The reaction rate constants \(k_f, k_r\) of the forward and reverse reaction are determined by the Arrhenius expression:
\[
k_j(T) = A_j T^{\beta_j} \exp \left( -\frac{E_{a,j}}{RT} \right)
\] (2.9)

where \(A_j, \beta_j\) are empirical coefficients and \(E_{a,j}\) is the activation energy which can be evaluated experimentally. The forward and reverse reaction rates are related through the equilibrium constant
\[
\frac{k_f}{k_r} = K_{c,j}
\] (2.10)

The total production or consumption rate of species \(\alpha\) is then
\[
\dot{\omega}_\alpha = \sum_{j=1}^{N} \dot{\omega}_{\alpha,j}
\] (2.11)

Putting all the relations together, one arrives at [34]
\[
\dot{\omega}_\alpha = W_\alpha \sum_{j=1}^{N} (v''_{a,j} - v'_{a,j}) A_j T^{\beta_j} \exp \left( -\frac{E_{a,j}}{RT} \right) \left[ \prod_{a=1}^{N} [X_a]^{v'_{a,j}} - \frac{1}{K_{c,j}} \prod_{a=1}^{N} [X_a]^{v''_{a,j}} \right]
\] (2.12)
2.1.3 Conservation of Momentum

Newton’s second law of motion states that the force acting on a system is equal the rate of change of its momentum. Furthermore, the force is divided into a surface force, represented by the stress tensor $\sigma_{ij}$, and a volumetric body force $f_{a,i}$.

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = -\frac{\partial \sigma_{ij}}{\partial x_j} + \rho \sum_{a=1}^{N} Y_a f_{a,i}$$  \hspace{1cm} (2.13)

where the stress tensor $\sigma_{ij}$ is expressed as:

$$\sigma_{ij} = \left[ p + \left( \frac{2}{3} \mu - \kappa \right) \right] \frac{\partial u_i}{\partial x_j} \delta_{ij} - \mu \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right]$$  \hspace{1cm} (2.14)

where $p$ is the hydrostatic pressure, $\mu$ denotes the dynamic and $\kappa$ the bulk viscosity and $\delta_{ij}$ is the Kronecker delta. Generally, $\kappa$ is neglected.

2.1.4 Conservation of Energy

The conservation equation for the total energy of the system, which includes the chemical, sensible and kinetic energies, one arrives at

$$\frac{\partial (\rho e)}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j e) = -\frac{\partial q_j}{\partial x_j} - \sigma_{ij} \frac{\partial u_i}{\partial x_j} + \rho \sum_{a=1}^{N} Y_a f_{a,i} U_{a,i}$$  \hspace{1cm} (2.15)

where $e$ contains both the sensible and chemical energies and $q_j$ denotes the heat flux vector. Furthermore, $q_j$ can be described as [34]:

$$q_j = -\lambda \frac{\partial T}{\partial x_j} + \rho \sum_{a=1}^{N} h_a Y_a U_{a,i}$$  \hspace{1cm} (2.16)

which represents conduction and mass diffusion heat transfer (from left to right). Here, second-order diffusion and radiation have been neglected [19].

2.1.5 Auxiliary Relations

The following auxiliary relations are needed in order to compute all the variables. The are found e.g. in [34].

**Ideal Gas Equation of State**

$$p = \frac{\rho R_a T}{\bar{W}} \quad \text{where} \quad \bar{W} = \sum_{a=1}^{N} X_a W_a = \frac{1}{Y_a W_a}$$  \hspace{1cm} (2.17)

**Energy-Enthalpy Relation**

$$h = \sum_{a=1}^{N} Y_a h_a = e + \frac{p}{\rho}$$  \hspace{1cm} (2.18)

**The Caloric Equation of State**

$$h_a = h_a^0(T^0) + h_a^e(T, T^0) \quad \text{where} \quad h_a^e(T, T^0) = \int_{T^0}^{T} c_{p,a} dT$$  \hspace{1cm} (2.19)

**Conversion between Molar and Mass Fractions**

$$X_a = \frac{Y_a / W_a}{\sum_{i=1}^{N} (Y_i / W_i)} \quad \text{and} \quad Y_a = \frac{X_a W_a}{\sum_{i=1}^{N} (X_i W_i)}$$  \hspace{1cm} (2.20)
2.2 Turbulence Modelling: Large Eddy Simulation

The objective of CFD-simulations is to calculate the quantities of interest and practical relevance of turbulent flows. At this point, the particular properties of turbulent flows have to be outlined. The velocity field $u(x,t)$ is three-dimensional, time-dependent and random. There is a large range of time and length scales. The largest turbulent motions are almost as large as the characteristic width of the flow and consequently affected by the system dimension. The smallest (Kolmogorov) length scale decreases as $Re^{-3/4}$ \[49\], i.e. the higher the Reynolds number, the smaller the Kolmogorov length scale. The Reynolds number is defined as the ratio of momentum forces to viscous forces and is a measure for the relative importance of these two, and therefore indicates the state of turbulence. It reads as:

$$Re = \frac{\rho u L}{\mu} = \frac{u L}{v} \quad (2.21)$$

where $\rho$ is the density, $u$ the characteristic velocity and $L$ the characteristic system dimension. The Navier-Stokes equations describe any type of flow, regardless if it was laminar or turbulent. As a part of their chaotic nature, no general solution is known, and only certain types of laminar flows can be solved analytically. Generally, turbulent flows have to be calculated numerically. To compute all relevant length and time scales, the Direct Numerical Simulation (DNS) is used. Since very fine meshes have to be employed and the range of length and time scales is tremendous, the time for computation scales with $Re^3$ and is restricted to certain cases where turbulence remains small. Therefore, other approaches than DNS have to be found in order to make computation of turbulent flows affordable. Many turbulence models have been proposed, such as the Reynolds-Averaged Navier-Stokes (RANS) approach, which is used to determine the mean velocity field ($\bar{u}$). It enjoys wide acceptance in the industry. Furthermore, in PDF methods a transport equation is solved for the evolution of the probability density function of the flow field $f(v;x,t)$. The last method to be mentioned here is the Large Eddy Simulation (LES), where the equations are solved for the filtered velocity field $\overline{u}(x,t)$, which is representative of the large-scale turbulent motions \[49\]. To capture the unsteady, highly turbulent nature of diesel sprays, the LES is the preferred method in this work.

![Figure 2.1: CFD grid with resolved and unresolved motions of the fluid flow. Red: energy-containing, non-universal scales which are captured and larger than the grid spacing. Blue: dissipative, universal sub-grid scales which need modelling.](image)

In LES, the larger three-dimensional unsteady turbulent motions (red in fig. 2.1) are directly represented, whereas the effects of smaller-scale motions (blue in fig. 2.1) are modelled. In terms of computational cost, LES is more expensive than the Reynolds’s stress models (e.g. $k-\epsilon$) and cheaper than DNS. Furthermore, the use of LES is motivated by the limits of either approach. For the well known RANS model, averaged momentum equations are used which lack the desired accuracy to describe large-scale unsteady flows. Because the energy-containing scales are represented explicitly in LES, it can be expected to be more reliable than Reynolds-stress models for...
flows in which large-scale unsteadiness is significant - such as the flow in diesel spray combustion for multiple injections [49]. On the other hand, in DNS nearly all the computational effort is used for the smallest, dissipative motions. Since the computational expense of DNS scales with the third power of the Reynolds number, it is usually not applicable for industrial purposes. That is where LES is advantageous again, the influence of the small scale, universal motions are represented by models and the dynamics of the large scale motions (which mainly contain the energy of the flow and are influenced by the system geometry) are computed explicitly which still leads to highly accurate simulations, dealing with lower cost compared to DNS.

2.2.1 Compressible, Filtered Navier-Stokes Equations

Filtering

To obtain the filtered Navier-Stokes equations, a general filtering operation has to be introduced where the integration is over the entire flow domain:

$$\overline{u}(x,t) = \int G(r,x)u(x-r,t)dr$$

This describes the convolution of the velocity field with the filter function $G$. The specific filter function $G$ needs to satisfy the normalization condition:

$$\int G(r,x)dr = 1$$

Therefore, the decomposition of the velocity field yields [49]:

$$u_i = \overline{u}_i + u'_i$$

which contains the filtered or resolved velocity and the residual or sub-grid velocity. It has to be outlined that $\overline{u}(x,t)$ resembles a random field and generally, the filtered residual is not zero (i.e. $u'_i \neq 0$) [49].

Favre Filtering

Most authors dealing with LES of compressible flows use a change of variable, in which filtered variables are weighted by the density. Mathematically, this change of variable is written as [24]

$$\Phi = \frac{\rho \Phi}{\rho}$$

Any scalar or vector variable can be decomposed into a low frequency part $\tilde{\phi}$ and a high frequency part $\phi''$, therefore

$$\phi = \tilde{\phi} + \phi''$$

If one compares the Favre decomposition to the Reynolds decomposition, where an arbitrary function is decomposed into a filtered quantity $\overline{\phi}$ and a residual quantity $\phi'$ ($\phi = \overline{\phi} + \phi'$), the following relations can be obtained:

$$\overline{\phi} - \tilde{\phi} = \frac{\rho \overline{\phi''}}{\rho} = -\frac{\rho \phi'}{\rho}$$

One can note the similarity to Favre averaging [27]. However, it is called Favre filtering, keeping in mind that it is in fact a filtering operation expressed in terms of Favre variables by a change of variable [24]. The motivation of using such an operator has two benefits:
1. The term \( \overline{\rho u_i} \) which is present after filtering the continuity equation (2.1) can be decomposed like in the following equation:

\[
\overline{\rho u_i} = \overline{\rho \hat{u}_i} + \text{sub-grid term} = \overline{\rho \hat{u}_i}
\]

(2.28)

which can easily be derived by equation (2.25). So the necessary transformation from \( \overline{\rho u_i} \) to \( \overline{\rho \hat{u}_i} \) would lead to another sub-grid term which can be avoided by transforming \( \overline{\rho u_i} \) to \( \overline{\rho \hat{u}_i} \) [24].

2. The Favre-filtered equations are structurally similar to their corresponding non-filtered equations, with exception of the sub-grid terms. Furthermore, the similarity with RANS is beneficial in terms of LES/RANS coupling [24]. As it is seen later on, this is a huge advantage, since the CMC combustion code was initially written for RANS approaches. Therefore, the transition to LES is facilitated.

**Formulation of the Filtered Governing Equations**

Due to the introduced Favre filtering, the continuity equation becomes:

\[
\frac{\partial \overline{\rho \hat{u}_i}}{\partial t} + \frac{\partial (\overline{\rho \hat{u}_i \hat{u}_j})}{\partial x_j} = 0
\]

(2.29)

The Favre filtered Navier-Stokes equations (momentum equations) are as follows [59]:

\[
\frac{\partial \overline{\rho \hat{u}_i}}{\partial t} + \frac{\partial \overline{\rho \hat{u}_i \hat{u}_j}}{\partial x_j} = -\frac{\partial \overline{\rho}}{\partial x_i} - \frac{\partial \overline{\rho \hat{u}_j R}}{\partial x_j} + \frac{\partial}{\partial x_j} (\overline{\delta_{ij} - \hat{\delta}_{ij}})
\]

(2.30)

where the stress tensor \( \sigma_{ij} \) is described as:

\[
\sigma_{ij} = 2\mu S_{ij} - \frac{2}{3} \mu \delta_{ij} S_{kk}
\]

(2.31)

and the rate-of-strain tensor

\[
S_{ij} = \frac{1}{2} \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)
\]

(2.32)

Moreover, the sub-grid scale (sgs) stress tensor defined as [24]

\[
\tau_{ij}^R = u_i \hat{\delta}_{ij} - \hat{u}_i \hat{u}_j
\]

(2.33)

and is unclosed, therefore it needs modelling and is discussed in the subsequent section.

**2.2.2 Sub-grid k or k-l model**

Since the Favre filtered momentum equation presents an unclosed residual stress tensor \( \tau_{ij}^R \), a closure is needed. It is obtained using an eddy viscosity model where the stress tensor is expressed as [9]

\[
\tau_{ij}^R = -2\nu_t \hat{S}_{ij} + \frac{2}{3} k_r \delta_{ij}
\]

(2.34)

where

\[
k_r = \frac{1}{2} \tau_{ii}^R
\]

(2.35)

is the residual turbulent kinetic energy and \( \nu_t \) is the turbulent viscosity. A transport equation for the sub-grid turbulent kinetic energy \( k_r \) is solved [9, 20, 7]:

\[
\frac{\partial k_r}{\partial t} + \frac{\partial j_{kr}}{\partial x_j} = -\tau_{ij}^R \hat{S}_{ij} - C_1 \frac{k_r^{3/2}}{\Delta} + \frac{\partial}{\partial x_j} \left( C_2 \Delta k_r^{1/2} \frac{\partial k_r}{\partial x_j} \right)
\]

(2.36)
where the sub-grid dissipation $\epsilon_r$ is defined as

$$\epsilon_r = C_1 \frac{k_r^{3/2}}{\Delta}$$  \hspace{1cm} (2.37)

Furthermore, the turbulent viscosity is modelled as a function of $k_r$:

$$\nu_t = C_2 \Delta k_r^{1/2}$$  \hspace{1cm} (2.38)

where the constants, $C_1$ and $C_2$, must be specified. Star-CD [9] uses values of $C_1 = 1$ and $C_2 = 0.05$.

### 2.2.3 Filter width

Performing LES using the commercial CFD software Star-CD (CD-adapco), a low-pass filtering operation is performed, so that the resulting velocity field $\tilde{u}_i$ is solved on a relatively coarse grid. The filter size $\Delta$ is generally equal to the mesh size [7]. In Star-CD it is defined as the filter width $\Delta$, which separates the resolved scales from sub-grid scales. In the finite volume discretisation, the filter width is clearly related to the mesh size [9]:

$$\Delta = \sqrt[3]{V}$$  \hspace{1cm} (2.39)

where $V$ is the cell volume. In the near-wall region, the energy-carrying eddies scale with the boundary layer thickness and therefore, the filter width is appropriately reduced by means of a mixing-length type damping function [9]:

$$\Delta = \min(\kappa y, \Delta)$$  \hspace{1cm} (2.40)

where $\kappa = 0.42$ and $y$ is the distance to the nearest wall. This ensures that eddy viscosity is effectively damped when $y$ tends to go to 0.

### 2.3 CMC Combustion Modelling

In non-premixed combustion, fuel and oxidizer are initially separated. Chemical reactions only occur after these two components have mixed. If the chemical reaction are fast enough, a reaction layer forms at stoichiometric conditions, where fuel and oxygen are consumed and reaction products are formed. In most engineering applications dealing with diesel-like fuels, combustion is typically controlled by the rate of molecular mixing. The chemistry only becomes important if the chemical time scale compares with the time scale of the turbulence which can lead to local flame extinction. To close any chemical source term, which appears in the averaged or filtered species transport equation in RANS or LES approaches, the so-called conserved scalar methods have been used in many applications. These methods have to be applied, since direct closure of terms, which incorporate chemical reaction rates coupled with turbulent fluctuations, can hardly be obtained. Conserved scalar method means that the rate of mixing of fuel and oxidizer has to be described by a non-reactive scalar, the mixture fraction. Essentially, the mixture fraction is a measure of the local equivalence ratio and hence, a conserved scalar which is independent of the chemistry. Detailed description of the mixture fraction concept can be found in [19]. If the sub-filter probability distribution of the mixture fraction is known, the Favre filtered mass fractions $\bar{\gamma}$ (or any other filtered value) can be obtained by [47]

$$\bar{\gamma} = \int_0^1 Q_\alpha \bar{P}(\eta) d\eta = \int_0^1 \bar{\gamma}_\alpha(\eta) \bar{P}(\eta) d\eta$$  \hspace{1cm} (2.41)

where $\eta$ is the mixture fraction in sample space and $\bar{P}(\eta)$ is the density-weighted filter probability density function (FPDF). The Conditional Moment Closure (CMC) is a conserved scalar model that accounts for finite rate chemistry effects and was derived in [3]. Like the PDF plays a central role in Reynolds-averaged (RANS) methods, it is the equivalent situation with the FPDF in LES.
In RANS approaches, a one-point PDF can be obtained by repeating an experiment several times and recording the mixture fraction at the position and time of interest, and accordingly, the PDF ensemble can be determined. In LES, one is only dealing with a single realization of the flow. Therefore, the unique properties observed at one specific location and time are not of statistical nature and hence, not enough to determine the FPDF. Therefore, the Filtered Density Function (FDF) is introduced which describes the local sub-filter state of a single realization. The FDPF is defined as the average of a sufficiently large number of samples of FDFs of the same resolved field.

Similarly like in RANS models, in LES a presumed shape of the FPDF has to be provided by a beta-function distribution. It is parametrized by the first two moments of the mixture fraction, namely the resolved (or filtered) mixture fraction $\tilde{\xi}$ and its sub-grid (or sub-filter) variance $\tilde{\xi}^{\text{sgs}}$. How these two are calculated is described in section 2.3.1. The beta-function is expected to be a better model for the FPDF in LES than PDF in RANS, because the FPDF is generally more narrow [47]. In the following section, the definition of the LES-CMC-equations and concepts are described.

2.3.1 Mixture Fraction Transport Equations

To obtain the resolved mixture fraction $\tilde{\xi}$, a transport equation has to be solved [57]:

$$\frac{\partial \tilde{\rho} \tilde{\xi}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{\xi} \tilde{u}_j)}{\partial x_j} = \frac{\partial}{\partial x_j} \left( \tilde{\rho} (D + D_t) \frac{\partial \tilde{\xi}}{\partial x_j} \right)$$

(2.42)

where $D_t$ is the turbulent diffusivity and a gradient model has been used to model the sub-grid scale flux:

$$\tilde{u}_j \tilde{\xi} = \tilde{u}_j \tilde{\xi} - D_t \frac{\partial \tilde{\xi}}{\partial x_j}$$

(2.43)

The transport equation is implemented in Star-CD and is solved internally. Furthermore, a transport equation is solved to obtain the sub-grid scale variance $\tilde{\xi}^{\text{sgs}}$:

$$\frac{\partial \tilde{\rho} \tilde{\xi}^{\text{sgs}}}{\partial t} + \frac{\partial (\tilde{\rho} \tilde{\xi}^{\text{sgs}} \tilde{u}_i)}{\partial x_i} = \frac{\partial}{\partial x_i} \left( \tilde{\rho} (D + D_t) \frac{\partial \tilde{\xi}^{\text{sgs}}}{\partial x_i} \right) - 2\tilde{\rho} \tilde{\chi} + 2\tilde{\rho} (D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i} \frac{\partial \tilde{\xi}}{\partial x_i}$$

(2.44)

where $\tilde{\chi} = D \frac{\partial (D + D_t) \frac{\partial \tilde{\xi}}{\partial x_i}}{\partial x_i}$ is the filtered scalar dissipation rate and is modelled as $\tilde{\chi} = \tilde{\chi}_{\text{res}} + \tilde{\chi}_{\text{sgs}}$, which is further investigated below. The nature of the sub-grid scale variance is that it decays by the effect of turbulence until mixing is complete, in which case it would be equal to zero. The diffusivity $D$ is calculated as the ratio of the molecular viscosity $\nu$ and the Schmidt number:

$$D = \frac{\nu}{S_c}$$

(2.45)

$D_t$ is the turbulent diffusivity and is discussed next. The turbulent diffusivity is $D_t$ is modelled as the ratio of the turbulent viscosity $\nu_t$ to the turbulent Schmidt number $S_c$, i.e. $D_t = \nu_t/S_c$. In this study, a constant value of $S_c = 0.9$ is used. The turbulent viscosity is obtained from equation 2.38.
The Scalar Dissipation Rate

The scalar dissipation rate of the mixture fraction is a fundamental parameter in non-premixed combustion which determines the filtered reaction rates, if combustion is mixing controlled. High rates of dissipation can also lead to local or global flame extinction [47]. The scalar dissipation rate measures species concentration gradients in the direction orthogonal to the flame, which incorporates the influence of the flow field on the local flame structure. Furthermore, it provides information about the mixing field and the combustion model (CMC). Figure 2.2 illustrates the regions having a high scalar dissipation rate.

Figure 2.2: Scalar Dissipation Rate visible in an example of diesel spray combustion.

The scalar dissipation rate may be decomposed into a resolved and a sub-grid scale (sgs) component for a closure [7]:

\[ \tilde{\chi} = \tilde{\chi}_{res} + \tilde{\chi}_{sgs} \]  
(2.46)

The resolved component can be evaluated from the filtered mixture fraction, where the molecular diffusivity is calculated as mentioned before:

\[ \tilde{\chi}_{res} = D \left( \frac{\partial \chi}{\partial x_i} \right)^2 = \nu \left( \frac{\partial \tilde{\chi}}{\partial x_i} \right)^2 \]  
(2.47)

while the unresolved component can be modelled as

\[ \tilde{\chi}_{sgs} = \frac{1}{2} \frac{C_s}{\Delta} \frac{\nu_t}{\Delta^2} \]  
(2.48)

where \( C_s \) is a constant which has to be determined. The term \( \nu_t/\Delta^2 \) has the unit of \( 1/s \), therefore the assumption can be be made that it is equal to a turbulent velocity time-scale \( \tau_t \) [28]. This time scale is computed using the filtered turbulent kinetic energy \( k_r \) and the filtered dissipation rate \( \epsilon_r \) which are outputs from Star-CD. Hence, the sub-grid scale scalar dissipation rate is computed as:

\[ \tilde{\chi}_{sgs} = \frac{\epsilon_r}{k_r} \frac{\nu_t}{\Delta^2} \]  
(2.49)

In the case of using a transport equation for the sub-grid turbulent kinetic energy \( k_r \), it becomes clear that the following condition must hold:

\[ \frac{\epsilon_r}{k_r} = C_1 \frac{k_r^{1/2}}{\Delta} \]  
(2.50)
where equation (2.37) was used. Replacing $k$ by the relation seen in equation (2.38), one arrives at

$$\frac{\varepsilon_r}{k_r} = \frac{C_1 v_l}{C_2 \Delta^2}$$  \hspace{1cm} (2.51)

Comparing equation (2.48) with (2.49), it can be seen that $C_x$ is equal to 40. This is similar to what was found in the literature ([23] used $C_N = 42$ and [7] used 50, keeping in mind that an algebraic model was used for the mixture fraction variance instead of a transport equation).

### 2.3.2 LES-CMC Formulation

In the following section, the equations for describing the turbulence-chemistry interactions in LES are described. The CMC combustion model belongs to the group of presumed PDF methods.

#### Conditional Filtering

Before the conditionally filtered equations can be derived, a suitable conditional filter needs to be introduced. This filter ensures consistency between the CMC-equations and the filtered Navier-Stokes equations that are solved in LES. A so-called fine-grained PDF is needed [39]

$$\psi_\eta = \delta[\xi(x,t) - \eta]$$  \hspace{1cm} (2.52)

where $\delta$ stands for a Dirac delta function and $\eta$ is the sample space of mixture fraction $\xi$. The fine-grained density is defined so that $\psi_\eta d\eta$ is the probability that at position $x$ and time $t$, $\xi$ will be in the range $\eta < \xi(x,t) < \eta + d\eta$ [57]. The conditional filtering procedure for the scalar $\phi$ then reads [39, 57]:

$$\bar{\phi}_{/\eta} = \frac{1}{V} \int_V \rho \phi \delta[\xi(x',t) - \eta] G(x - x', \Delta) dx'$$

$$\phi$$ can either be replaced by the mass fraction $Y_\alpha$ of species $\alpha$ or enthalpy $h$. $G$ is a positive filter function with filter width $\Delta$, $V$ is the control volume of a computational cell and $\bar{P}(\eta)$ is a density-weighted filtered probability density function (FPDF) [57]

$$\bar{\phi}_{/\eta} = \frac{1}{\hat{\rho}} \int_V \rho \delta[\xi(x',t) - \eta] G(x - x', \Delta) dx'$$

and has all the properties of a PDF. The unconditional, filtered value can be obtained by integration of the conditional value over $\eta$-space:

$$\hat{\phi} = \int_0^1 \hat{\phi}_{/\eta} \bar{P}(\eta) d\eta$$

However, since in LES-CMC a presumed shape of the FPDF has to be provided via a beta-function distribution, the filtered probability density function is assumed to be [57]

$$\bar{P}(\eta) = \frac{\eta^{\alpha-1}(1-\eta)^{\beta-1}}{B(\alpha, \beta)}$$

where

$$B(\alpha, \beta) = \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha + \beta)}$$

is the beta-function and $\Gamma(x)$ is the gamma-function. The parameters $\alpha$ and $\beta$ depend on the mixture fraction only:

$$\alpha = \frac{\bar{\xi}(1-\bar{\xi})}{\bar{\xi}^{\mu_2} - 1} \quad \text{and} \quad \beta = \frac{\alpha (1-\bar{\xi})}{\bar{\xi}}$$

$$\bar{\xi}$$
2.3.3 CMC equations

Filtering of the transport equations for the scalar $Y_\alpha$, and introducing $Q_\alpha = \overline{Y_\alpha \mid \eta} = \rho \overline{Y_\alpha / \rho_\eta}$ as the conditionally filtered reactive scalar, leads to [57]

$$\frac{\partial Q_\alpha}{\partial t} + u_i \frac{\partial Q_\alpha}{\partial x_i} = \chi \frac{\partial^2 Q_\alpha}{\partial \eta^2} + \omega_\alpha + e_f$$  \hspace{1cm} (2.59)

where $\overline{u_i \mid \eta}$ is the conditionally filtered velocity, $\overline{\chi \mid \eta}$ the conditionally filtered scalar dissipation rate, $\overline{\omega_\alpha \mid \eta}$ is the conditionally filtered reaction rate and the term

$$e_f = \frac{1}{\bar{\rho} \bar{P}(\eta)} \frac{\partial}{\partial x_i} \left( \bar{\rho} \bar{P}(\eta) D_i \frac{\partial Q_\alpha}{\partial x_i} \right)$$  \hspace{1cm} (2.60)

is the sub-grid scale conditional flux. The term $e_f$ accounts for the conditional transport in physical space where a gradient model was used [57]. However, a number of terms of equation (2.59) need modelling.

Conditional Velocity

Since linear models for the conditional velocity have only been validated for Reynolds-Averaged Navier Stokes models, the use of a constant value for $\overline{u_i \mid \eta}$ has been proposed for LES [57]:

$$\overline{u_i \mid \eta} = \tilde{u}_i$$  \hspace{1cm} (2.61)

where $\tilde{u}_i$ is the unconditional, filtered velocity.

Conditionally Filtered Scalar Dissipation Rate

The Amplitude Mapping Closure (AMC) is a method to use the conditionally filtered dissipation rate [40, 57]:

$$\overline{\chi \mid \eta} = \chi_0 G(\eta)$$  \hspace{1cm} (2.62)

where $G(\eta)$ is the error function (not to confuse with the filter function)

$$G(\eta) = exp(-2[erf^{-1}(\eta - 1)]^2)$$  \hspace{1cm} (2.63)

and

$$\chi_0 = \frac{\tilde{\chi}}{\int_0^1 \bar{P}(\eta) G(\eta) d\eta} = \frac{\tilde{\chi}_{res} + \tilde{\chi}_{sgs}}{\int_0^1 \bar{P}(\eta) G(\eta) d\eta}$$  \hspace{1cm} (2.64)

Conditionally Filtered Reaction Rate

For the conditionally filtered reaction rate $\overline{\omega_\alpha \mid \eta}$, a first order closure is provided where the conditionally filtered reacting scalars are used for calculation:

$$\overline{\omega_\alpha \mid \eta} = \omega_\alpha(Q_1, Q_2, \ldots, Q_n)$$  \hspace{1cm} (2.65)

where $n$ is the number of reacting scalars. The effective equation for the conditionally filtered reaction rate is dependent on the employed reaction mechanism.
2.4 CMC Multiple Injections Formulation

Contionally Filtered Enthalpy Equation

The conditionally filtered enthalpy can be defined as \( Q_h = \overline{h}\eta \) and therefore, similarly to the conditional species equations (2.59), it reads [39]

\[
\frac{\partial Q_h}{\partial t} + u_i \frac{\partial Q_h}{\partial x_i} = \chi \frac{\partial^2 Q_h}{\partial \eta^2} + q \frac{\partial \eta}{\partial t} + \epsilon_h \tag{2.66}
\]

where the two new terms are the conditional heat flux \( q\eta \) and the term \( \epsilon_h \), which describes the correlation of the conditional fluctuations and the scalar \( h \). These two terms may be closed in similar fashion as in the species equations.

Chemico-thermal enthalpy

Heat transfer in Star-CD is implemented by the following form of the enthalpy transport equation for a fluid mixture [9]:

\[
\frac{\partial \tilde{p}h}{\partial t} + \frac{\partial}{\partial x_j} (\tilde{p}uh_j + F_{h,j}) = \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_j}{\partial x_j} + s_h \tag{2.67}
\]

Here, \( h \) is the filtered static enthalpy which is defined as:

\[
h = \sum_{a=1}^{N} h_a \tilde{Y}_a = \sum_{a=1}^{N} \left( \int_{T^0}^{\tilde{T}} c_{p,a}(T) \tilde{Y}_a dT + h_a^{T} \tilde{Y}_a \right) = c_p \tilde{T} \tag{2.68}
\]

Furthermore, in equation (2.67), \( F_{h,j} \) is the diffusional energy flux in direction \( x_j \), \( s_h \) is the energy source and \( \tau_{ij} = 2\mu \delta_{ij} - 2\mu \frac{\partial u_k}{\partial x_i} \delta_{ij} \) is the matrix of the stress tensor components. In terms of coupling Star-CD and CMC, the energy source (chemical energy) is an output from CMC and therefore, the chemico-thermal enthalpy equation can be transported by Star-CD employing polynomial \( c_p \) for species. As a result, the unconditional temperature can be calculated.

2.4 CMC Multiple Injections Formulation

In literature [26, 16, 11, 12], considerable effort has been put into increasing the dimensionality of flamelet models in order to account for more than one spray in the sense of multiple injections. The Representative Interactive Flamelet (RIF) model was modified to accommodate the two-dimensional flamelet equations and two mixture fractions [26], slightly later it was extended to allow any number of injections [16]. These methods basically describe a three-feed system in which more than two streams are mixing and the basic equations are depending on mixture fractions \( e_1 \) and \( e_2 \). Extending the dimensionality of the CMC equations would lead to a tremendous increase of complexity and therefore computational costs. Hence, an extended Conditional Moment Closure model has been introduced [5] in a RANS context and has successfully been applied [18, 41], which can account for an arbitrary number of subsequent injections. The model has been described as a sequential two-feed system rather than a three-feed system where the total mixture fraction (MFT=MF1+MF2) is used as the conditioning scalar. This is motivated due to the fact that a rapid transition from the 2D flamelet space into a quasi-1D flamelet along the MFT coordinate is estimated after the second injection has started (e.g. seen in [16]). Since the structure of RANS-CMC equations and LES-CMC equations are alike, the multiple injection approach developed for RANS can be adapted to the LES case. The main idea of the model is to transform the original temperature and species profiles conditional on the mixture fraction originating from the first injection (MF1) into representative profiles which are conditional on the total mixture fraction (MFT). It has to be pointed out that using one conditional quantity instead of two requires the collapse of one dimension similar to what is seen during initialisation of a 2D-RIF model in case of a subsequent injection [16]. Since the CMC grid is spatially resolved in two dimensions, a
detailed determination of the time and location of the contact between fuel streams as well as their local conditions is possible. The model is based on reinitialization of the conditional temperature and species profiles in every CMC cell at the time of the first appearance of the of the mixture fraction coming from the second fuel stream (MF2). For the sake of brevity, the reinitialization is explained for the temperature profile only, but in the same fashion it can be applied on any species profile. At the time of first MF2 appearance, it is proposed to introduce the doubly conditioned temperature distribution which is exemplarily drawn in 2.3 a).

![Example of a doubly conditioned temperature distribution at the time of reinitialization (18)](image1)

![Combined conditional temperature profile (17)](image2)

Figure 2.3: Temperature profile resulting from combining old temperature profile in MF1 space with the new temperature profile in MF2 space.

The reinitialization procedure is based on two basic assumptions: 1) at the instant of the first MF2 appearance in a CMC cell, MF1 (ε1) and MFV1 (ε2) only tend to decrease due to convection-diffusion effects and due to the absence of an MF1 source (e.g. the first injection has ended). This implies that the sources of MF1 and MF2 (e.g. the first and second injection) need to be separated in time and cannot overlap each other. Since a given MF1 value in a CMC cell only tends to decrease, only the left part of the temperature profile has a physical meaning and has to be retained (seen as the black line in 2.3 b)). At later stages of combustion, higher values of MF1 are not expected to exist. 2) As soon as the second fuel stream enters a cell, the increase of MFT is attributed to MF2 only, i.e. the right part of the temperature profile has to be recreated in order to account for the second mixture fraction (seen as the red line in 2.3 b)). For the ease of comprehension, a single value of 0.06 for MF1 in a CMC cell is considered. Therefore, looking at 2.3 a), the horizontal arrow (MF2=0) corresponds to the existing burning profile caused by MF1 and the vertical arrow (MF1=const.) corresponds to adiabatic mixing (i.e. no chemical interaction between MF1 and MF2 is assumed at the onset). Note that MF1+MF2 cannot exceed 1 (pure fuel), therefore the domain is a unity triangle.

The new recreated temperature profile can be described by the following expression:

\[
\tilde{T}_{\text{Double}}[\eta_1, \eta_T] = \tilde{T}_{\eta_1}[\eta_T] \left[ H(\eta_T) - H(\eta_T - \eta_1) \right] + \tilde{T}_{\text{Mix}}[\eta_T] H(\eta_T - \eta_1)
\]

(2.69)

where \( \eta_T \) is MFT, \( \eta_1 \) is the the local value of MF1 in the CMC cell when new fuel enters the control volume, \( \tilde{T}_{\eta_1}[\eta_T] \) is the existing conditional temperature profile in the CMC cell before reinitialization and \( \tilde{T}_{\text{Mix}}[\eta_T] \) is the adiabatic mixing temperature profile obtained following the \( \eta_2 \) coordinate for \( \eta_1 = \text{constant} \) on the doubly conditioned temperature distribution. \( H(\eta) \) is the Heaviside step function which is defined as:
18

4. CMC Multiple Injections Formulation

\[ H(\eta) = \begin{cases} 0 & \text{if } \eta < 0 \\ 1 & \text{if } \eta \geq 0 \end{cases} \]  

(2.70)

At the moment when MF2 arrives in a new CMC cell the reinitialization follows instantaneously without having a MF2 value in the control volume. Therefore, the marginal FPDF \( \overline{P}_{T_1|\xi}(\eta_1|\eta) \) is assumed to be the current MF1 FPDF \( \overline{P}_{T_1}(\eta_1) \). The new temperature profile conditional on MFT, \( \overline{T_{New}|\eta_T} \) is obtained by convolution of the double conditional temperature (2.69) and the FPDF of MF1 [18]:

\[
\overline{T_{New}|\eta_T} = \int_0^1 \overline{T_{Double}|\eta_T, \eta_T} \overline{P}_T(\eta_1) \, d\eta
\]

(2.71)

The reinitialization process described above is depicted in figure 2.4, where the thick black line is the original profile before MF2 enters the domain and the several thin black lines represent reinitialized temperature profiles for different values of MF1. To illustrate the influence of the MF1 FPDF, three different cases are shown in figure 2.4: a low resolved MF in connection with a high (green) and a low (blue) MFV and a high resolved MF in with a low MFV (red). The temperature profile that corresponds to an MF1 FPDF is drawn in the same colour. The collapse after reinitialization follows and the conditioning variable is MFT instead of MF1. Now it gets clear that for low MFV (blue and red curves), the temperature profile converges to a single cut at the specific MF1 value, whereas for high MFV (green curve) the profiles get more rounded. Moreover, it has to be noted that the profiles are differentiable and continuous [18].

![Figure 2.4: Re-initialized temperature profiles for different distributions of MF1 [18]. The temperature profile that corresponds to an MF1 FPDF is drawn in the same colour. The collapse after reinitialization follows and the conditioning variable is MFT instead of MF1 (x-axis).](image)

Having the reinitialized temperature profile, the computation of unconditional quantities (i.e. \( \overline{T}, \overline{Y_a} \)) follows, as it is common in the CMC framework, by convolution of the new profiles with the MFT FPDF, which is found by solving transport equations for the resolved and the sub-grid scale variance of the total mixture fraction. The initialization process is a local effect which is then transported in physical as well as in conserved scalar space. The number of subsequent injections is not limited, given that the injections are separated in time. In fact, the temperature and species profiles only need to be reinitialized before a new injection [18].
2.5 Direct Integration

The are some main differences between the CMC model and Direct Integration model (DI). First of all, DI considers the computational control volume as well-mixed, whereas the CMC model assumes the mixture fraction to be distributed as a $\tilde{\beta}$-PDF. Secondly, CMC includes the Scalar Dissipation Rate (SDR) which is an important parameter representing molecular mixing, a phenomenon which is missing in the DI formulation. If the SDR is high, auto-ignition is delayed or even inhibited. In the limiting case of zero mixture fraction variance and zero SDR, the CMC model converges to the well-mixed case implying a $\delta$-function for the mixture fraction distribution and no small-scale mixing effects [4].

2.6 Models for Atomization and Secondary Break-Up

Since a diesel injection contains liquid fuel that is injected into a high pressure and temperature air field, one has to consider multi-phase flow. In Star-CD, dispersed multi-phase flow are treated with Lagrangian/Eulerian models, where the continuous phase is the air and the dispersed phase are the liquid fuel droplets. The two phases strongly influence each other via displacement and transfer of momentum, mass and heat. The conservation equations of mass, momentum and energy for the dispersed phase are written for each individual element if the number of particles is low, whereas a statistical approach is used for a large number of particles. On the other hand, the governing equations for the carrier phase are expressed in Eulerian form and take account for the dispersed phase [9].

First of all, the interaction of a single droplet with the surrounding gas phase (i.e. air) is described by laws of momentum (drag/aerodynamic forces), mass and energy (evaporation) exchange mechanisms [61].

2.6.1 Aerodynamic Forces

The drag force of a spherical droplet in a gaseous surrounding is [9]

$$ F_{drag} = \frac{1}{2} C_{drag} \rho A_d |u - u_d|(u - u_d) $$

(2.72)

where the drag coefficient $C_{drag}$ can be described as [9]

$$ C_{drag} = \begin{cases} 24(1 + 0.15Re_{d}^{0.687})/Re_{d} & , \quad Re_{d} \leq 10^3 \\ 0.44 & , \quad Re_{d} > 10^3 \end{cases} $$

(2.73)

and $Re_{d}$ is the droplet Reynolds number, defines as [9]

$$ Re_{d} = \frac{\rho |u - u_d| D_d}{\mu} $$

(2.74)

Here, $\mu$ is dependent on temperature and $D_d$ is the droplet diameter.

2.6.2 Evaporation

In order to evaporate a liquid droplet, mainly two effects are important. On one hand, the mass transfer at a rate $F_m$ per unit surface area, the droplet mass rate of change is given by [9]

$$ \frac{d m_d}{dt} = -A_s F_m $$

(2.75)

where $A_s$ is the droplet surface area. For an evaporating droplet, $F_m$ can be described as [9]

$$ F_m = K_e p_t \ln \frac{p_t - p_{v,inf}}{p_t - p_{v,s}} $$

(2.76)
where \( p_t \) is the gas pressure, \( p_{v,\text{inf}} \) and \( p_{v,s} \) are the partial pressures of the vapour in the droplet surroundings and at its surface, respectively. The surface vapour pressure \( p_{v,s} \) is assumed to be equal to the saturation pressure at the droplet temperature \( T_d \). Furthermore, \( K_g \) is the mass transfer coefficient and is obtained using the Sherwood number

\[
Sh = 2 \left( 1 + 0.3 \frac{Re_d^{1/2} Sc^{1/3}}{Sc} \right)
\]

where \( Sc \) is the Schmidt number. The mass transfer coefficient \( K_g \) is defined as [9]:

\[
K_g = \frac{Sh D_m}{R_m T_m D_d}
\]

where \( R_m \) is the mixture gas constant, \( D_m \) is the vapour diffusivity and \( T_m \) the mean (film) temperature [9].

On the other hand, the droplet energy balance takes two effects into account: Firstly the mechanism of surface heat transfer rate \( \dot{q}_d'' \) per unit surface area and secondly the loss/gain due to phase change, thus [9]:

\[
m_d c_{p,d} \frac{dT_d}{dt} = -A_d \dot{q}_d'' + h_{fg} \frac{dm_d}{dt}
\]

where \( A_d \) is the droplet surface area, \( c_{p,d} \) the droplet specific heat and \( h_{fg} \) the latent heat of phase change. The heat flux of the surface is defined as the convective heat transfer [9]:

\[
\dot{q}_d'' = h(T_d - T)
\]

The heat transfer \( h \) coefficient be calculated by [9]

\[
h = \frac{k_m Nu Z}{(e^Z - 1) D_d}
\]

where the Nusselt number (\( Nu \)) is obtained from [9]

\[
Nu = 2 \left( 1 + 0.3 \frac{Re_d^{1/2} Pr^{1/3}}{Pr} \right)
\]

in which \( Pr \) is the Prandtl number. The value \( Z \) is defined as [9]

\[
Z = \frac{-c_p \frac{dm_d}{dt}}{\pi D_d k_m Nu}
\]

Here, \( k_m \) is the fluid conductivity of the carrier phase [61].

### 2.6.3 Atomization

In an engine combustion chamber, the liquid fuel enters through an injection nozzle. In order to determine the droplet properties, a full simulation of the injection system would be necessary including the transient injection needle motion and nozzle discharge. Since the nozzle diameter and the relevant dimensions of the injector are usually orders of magnitudes smaller than the combustion chamber, a significant amount of computational power would be required to simulate the nozzle opening and the fuel injection. Therefore, the droplet properties at the nozzle exit are prescribed by models. These models take into account nozzle specific information and can be viewed as boundary conditions in the solution domain [61].
Reitz and Diwakar Model

Many different atomization models are existing, whereas the Reitz and Diwakar atomization (R-D) was used in the scope of this project for the reason that it showed accurate results in non-reactive simulations [63]. The spray angle is an input value and needs to be specified in advance. Based on this angle (see figure 2.5), the initial droplet velocity is determined according to [9] (page 12-27). In the model, the liquid core is represented by a chain of primary droplets (spheres) which have the initial diameter equal to the nozzle diameter [9]. According to [50, 9], droplet break-up occurs due to aerodynamic forces and in one of the following modes:

1. Bag break-up: The non-uniform pressure field around the droplet causes it to expand, which causes disintegration if the surface tension forces are overcome.

2. Stripping break-up: Liquid is sheared or stripped from the droplet surface.

A closer description of the Reitz and Diwakar model can be found in the Star-CD manual [9].

![Figure 2.5: Detailed picture of an injected diesel spray](image)

2.6.4 Secondary Droplet Break-Up Models

The liquid fuel core (seen in figure 2.5) enters at a velocity of several hundred meters per second into the combustion chamber which is filled with quiescent air. The sides and the tip of the spray are exposed to tremendous shear stresses, which causes the liquid core to break up into smaller fuel droplets. Since the combustion chamber is representative for a diesel engine at top dead centre (TDC), high temperature (900 K) and pressure (60 bar) are met, which cause high heat transfer rates and therefore fast evaporation. The phenomenon of droplet break-up is described with different models. As it was seen in [63], different models were evaluated to simulate a split injection by LES. Comparison of the simulated data with the experimental results from Skeen et al. [55] led to the conclusion that the Kelvin-Helmholtz and Rayleigh-Taylor (KHRT) droplet break-up mechanism performed best for the present setup.

KHRT

The Kelvin-Helmholtz (KH) and Rayleigh-Taylor (RT) droplet break-up model was described by Patterson and Reitz [42] and consists of two simultaneously computed processes which are competing against each other. The KH process detects instabilities growing on a droplet surface where small droplets are shed. The RT instabilities result from the deceleration of the injected droplets and cause a complete break-up of the droplets into new droplets of different sizes. The process that predicts the fastest onset of an instability causes a break-up event. The model equations can be found e.g. in [9] (chapter 12).
2.6.5 Summary

In figure 2.6, a characteristic process is visible where the effects of atomization, droplet break-up and evaporation interact with each other. It needs to be emphasized that this is not the injection of particular interest of the project, but helps to understand the process and is only shown exemplarily. The depicted process shows the time evolution of the distribution of droplets in the combustion chamber. Large, unbroken droplets remain in the region near the nozzle. The high shear stresses acting on the sides of the spray strips the droplets apart, leading to smaller droplets that evaporate fast due to high heat transfer to the surroundings.

Figure 2.6: Time evolution of a fuel spray in a nitrogen filled cylindrical chamber at 11 bar [2]. Initially, the gas-phase in the chamber is at rest.
Chapter 3

Experimental Setup

All experiments mentioned in this report were conducted at the Combustion Research Facility, Sandia National Laboratories, Livermore CA. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy’s National Nuclear Security Administration [55]. The Engine Combustion Network (ECN) group has identified several standard experimental conditions to which modellers worldwide can refer to, so the findings can be compared to each other. The ECN group has agreed to use the same injector and ambient conditions in the experiments, which is made possible by the donation of "identical" injection systems by Robert Bosch LLC [52]. This work is mainly focused on reproducing the split injection experiment of Skeen et al. [55]. A detailed overview of the experimental findings can be found in the beforehand referenced paper.

3.1 Spray A Conditions

One injection setup is the so-called "Spray A". It includes high and low temperature combustion conditions relevant to engines that use moderate Exhaust Gas Recirculation (EGR). It uses a modern and advanced injection system with high pressure capability. The detailed specifications for the two Spray A operating conditions of the ECN, which were investigated, can be found in table 3.1. The experimental ambient gas conditions resemble engine operating conditions. Like it was already mentioned, two cases have been considered for this study: 900 K as the diesel-like (referred to as "Case 1") and 750 K as the LTC-like (referred to as "Case 2") operating conditions. 15 % oxygen was used to investigate ignition and combustion phenomena and 0 % oxygen (i.e. non-reactive) was used to characterize mixing and vapour penetration length without effects of heat release [55]. ECN has proposed a Spray A split-injection schedule with 0.5 ms injection, 0.5 ms dwell and 0.5 ms injection and is illustrated in figure 3.1. The modelled rate of injection used for CFD modelling is available from [33].

3.2 Combustion Chamber Geometry

The nearly cubical pre-burn combustion vessel has approximately a volume of 1 litre and is depicted in figure 3.2. Sprays of n-dodecane are directly injected into the combustion chamber. The fuel injector is mounted in the middle of one face so that the spray is directed to the centre of the chamber. Four transparent windows allow for optical access [55]. A mixing fan and two spark plugs are mounted at another face.

The procedure of injection experiment is as follows. Prior to an experiment, the vessel is heated to 458 K before a certain amount of premixed, combustible gas is spark ignited by the two spark plugs to produce consistent combustion in the high-density, fuel-lean environment [31]. This premixed combustion creates a high temperature and high density environment. The mixing fan runs throughout the whole experiment and ensures to have a uniform temperature distribution inside.
Table 3.1: Spray A, experimental conditions [52]

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient gas temperature</td>
<td>900 K / 750 K</td>
</tr>
<tr>
<td>Ambient gas pressure</td>
<td>59.8 bar / 49.3 bar</td>
</tr>
<tr>
<td>Ambient gas density</td>
<td>22.8 kg/m³</td>
</tr>
<tr>
<td>Ambient oxygen content (by volume)</td>
<td>15% O₂ (reacting)</td>
</tr>
<tr>
<td></td>
<td>0% O₂ (non-reacting)</td>
</tr>
<tr>
<td>Nominal nozzle diameter</td>
<td>0.090 mm</td>
</tr>
<tr>
<td>Discharge coefficient C_d</td>
<td>C_d = 0.86</td>
</tr>
<tr>
<td>Fuel injection pressure</td>
<td>1500 bar, before SOI</td>
</tr>
<tr>
<td>Fuel (diesel surrogate)</td>
<td>n-dodecane (C₁₂H₂₆)</td>
</tr>
<tr>
<td>Fuel temperature</td>
<td>363 K (90°C)</td>
</tr>
<tr>
<td>Injection duration</td>
<td>0.5 ms/ 0.5 ms dwell / 0.5 ms</td>
</tr>
<tr>
<td>Injected fuel mass</td>
<td>1ˢᵗ: 1.18 mg, 2ⁿᵈ: 1.16 mg</td>
</tr>
</tbody>
</table>

Figure 3.1: Measured and modelled rate of injection for the split injection setup [33].

The average swirl velocity is approximately 0.7 m/s, compared to the high injection velocities (~ 400 – 600 m/s) it only has little effect on the sprays and can therefore be neglected. In a second step, the combustion products cool down (over a period of ~ 1 s) and the pressure slowly decreases [30]. At the instant when the desired experimental conditions are reached, the diesel fuel surrogate is injected and the non-premixed combustion of interest takes place. An exemplary cool down of such an experiment (not for 900 K) is shown in figure 3.3.

3.3 Optical Diagnostics

Two methods of optical diagnostics have been applied for this study and use the same perspective for direct comparison. The first is planar laser-induced fluorescence (PLIF) and the second is schlieren imaging.

**PLIF:** Laser (355 nm wave length) is shot along a thin plane of the fuel jet to excite formaldehyde fluorescence. Formaldehyde PLIF can possibly suffer from interference due to polycyclic aromatic hydrocarbons (PAH) fluorescence as well as laser-induced incandescence (LII) from soot. However, to a certain extent it can be distinguished from formaldehyde PLIF temporally and spatially (which
is rather difficult for the second injection though. It is noteworthy that formaldehyde PLIF yields a lower intensity than that attributed to PAH. For the diesel-like condition (900 K) soot is estimated and interference poses a problem whereas for the LTC-like condition soot formation is not expected [55].

**High-speed schlieren imaging:** With the schlieren imaging techniques it is possible to visualize the vapour penetration length, first-stage ignition and second-stage ignition due to the variability of density. The high-speed imaging camera is able to capture 150'000 frames per second.

---

**Figure 3.2:** Combustion vessel geometry and configuration [32].

**Figure 3.3:** Exemplary cool down procedure for ambient conditions 1000 K, 14.8 kg/m³, 21 % O₂. Illustrated is the pressure evolution [30].
Chapter 4

Numerical Setup

4.1 Flow Field Solver (CFD)

Simulations have been carried out using the commercial CFD-solver Star-CD [9] coupled with an elliptic first-order CMC combustion model [6, 21, 60]. The turbulent flow field is solved by the LES turbulence model using an additional transport equation for the sub-grid turbulent kinetic energy ($k_r$). In figure 4.1, the 3D-CFD mesh is visible. The computational mesh is adopted from Farrace et al. [14], in which context it was successfully applied for the simulation of Spray A single injections. The CMC grid is superimposed, however its resolution still has to be determined (i.e. 1D or 2D-CMC) and is therefore not shown. The computational domain resembles a diesel engine at top dead centre conditions met in the constant volume combustion chamber from the previous chapter 3. The CFD mesh possesses different refinement regions (seen in table 4.1) and contains approximately 1.9 million cells. The two-phase flow field is solved by the built-in Lagrangian/Eulerian formulation. The atomization was modelled using the Reitz-Diwakar model [50] and the secondary droplet break-up by the Kelvin-Helmholtz and Rayleigh-Taylor model [42]. The droplet drag as well as heat and mass transfer is computed using the standard implementations of Star-CD which have been presented before. Further details and references of the particular models can be found in [9]. Star-CD internally calculates the thermo-physical droplet properties (such as density, viscosity, $c_p$, latent heat, surface tension and vapour pressure) of $n$-dodecane as a function of temperature [13]. The transport equation for the chemico-thermal enthalpy are solved by Star-CD where polynomials for the different species are employed.

4.2 CMC Code

The CMC model is a presumed PDF method. As it is a common approach in the non-premixed combustion, the mixture fraction is used as the conditioning variable, since it is a conserved scalar. The governing equations have already been presented in chapter 2. The transport equations for conditionally filtered species and enthalpy are solved in each CMC cell. The CMC equations are discretized with finite differences, where a second order scheme is used for the diffusion terms in both conserved scalar and physical space and a first order upwind scheme to compute the convective terms [13]. Furthermore, the stiff integrator ISAT (In Situ Adaptive Tabulation [48]) is used for time integration, while a full operator splitting technique (OS) is applied. The implementation of OS separates the stiff, chemical part of the system from the non-stiff convection-diffusion part. So in a first step, the physical-space transport is computed followed by a second step solving together the reaction and diffusion in the conserved scalar space part of the whole CMC equation. There are mainly two advantages coming along with OS, firstly, the number of simultaneously solved ODEs is reduced and secondly, the possibility of using different solvers arises for each time step depending on the characteristics of the ODE system [60]. Furthermore, the mixture fraction is discretized into 101 computational nodes clustered around the stoichiometric value.
Since the spatial fluctuations of conditional quantities are much weaker than their unconditional (Favre filtered) values, a coarser spatial resolution can be applied for the CMC grid compared to the CFD mesh. Furthermore, it has been shown that a two-dimensional formulation of the CMC-equation shows appropriate results for diesel simulations [13]. This is common practice and means that cells in azimuthal direction are collapsed and therefore, all circumferential CFD information is reduced into one CMC cell and the CMC equations are solved axially and radially. Hence, a 2D-CMC-grid was used for this study, whereas the CFD mesh is three-dimensional which is necessary to perform LES. Since one CMC-cell can contain multiple CFD-cells, integration in space is required to transfer information from one grid to another. Integrating the conditionally filtered random variable \( f \) over the volume \( V_{CMC} \) of a CMC cell yields [57]:

\[
\bar{f} \sim [\eta^*] = \frac{\int_{V_{CMC}} \hat{P}(\eta) dV'}{\int_{V_{CMC}} \hat{P}(\eta) dV'}
\] (4.1)

Equation (4.1) explains that quantities which are required at the coarser CMC grid resolution (e.g. scalar dissipation rate or conditional velocities) are obtained by FPDF weighted volume averaging of the respective quantities, found from cells at the corresponding locations of the finer CFD grid. The unconditional filtered species mass fractions \( \bar{Y}_\alpha \) are calculated by convolution of the conditionally filtered quantity \( Q_\alpha \) with the \( \beta \)-FPDF in each CFD cell [13]. A schematic of the interaction between the CFD-solver and the CMC code is shown in figure 4.3.

### 4.3 Additional Numerical Considerations

The computational effort of an LES-CMC simulation is closely connected to the employed chemical reaction mechanism. In the skeletal mechanism of Yao et al. [62], 54 species and 269 reactions are introduced. Therefore, a high amount of transport equations have to be solved: 3 momentum equations, 1 enthalpy equation, 2 equations for the resolved mixture fractions MFT and MF2 and 1 for the mixture fraction variance on the relatively fine LES grid and 54 species plus 1 enthalpy equation on the relatively coarse CMC grid, which makes a total number of 62 transport equations which are solved at a constant time step of 0.5 \( \mu s \). This corresponds to Courant numbers between 0.4 and 2.4. A characteristic evolution of the Courant number is shown in figure 4.2. The mathematical definition of the Courant or CFL (Courant–Friedrichs–Lewy) number is as follows

\[
C = \Delta t \left( \frac{u_1}{\Delta x} + \frac{u_2}{\Delta y} + \frac{u_3}{\Delta z} \right)
\] (4.2)

The principle behind this condition is if e.g. a pressure wave is moving over discrete points of the computational grid and we want to calculate its amplitude at discrete time steps of equal duration, then this duration must be less than the time for the wave to travel to the next grid point [10]. This is generally true for explicit methods. In the current setup however, an implicit method is used, therefore the condition is less restrictive and also larger values may be tolerated, since it is less sensitive to numerical instability. A Courant number of approximately 2 was chosen to be appropriate in [15], therefore a constant time step of 0.5 \( \mu s \) was chosen to be reasonable in combination with the mentioned CFD mesh.
Figure 4.1: Mid-planar section of the computational domain. The Cartesian grid contains 5 different refinement regions seen in detail in the table below. The contour plot of the spray is shown exemplarily at 2.0 ms ASOI.

Table 4.1: Refinement regions of the computational CFD mesh (from figure 4.1) adopted from [14].

<table>
<thead>
<tr>
<th>Mesh refinement zone</th>
<th>x,y - directions (mm)</th>
<th>z - directions (mm)</th>
<th>Cell size $V^{1/3}$ (mm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0-3</td>
<td>0-40</td>
<td>0.125</td>
</tr>
<tr>
<td>2</td>
<td>3-4</td>
<td>0-60</td>
<td>0.25</td>
</tr>
<tr>
<td>3</td>
<td>4-14</td>
<td>0-108</td>
<td>0.5</td>
</tr>
<tr>
<td>4</td>
<td>14-26</td>
<td>0-108</td>
<td>1.0</td>
</tr>
<tr>
<td>5</td>
<td>26-54</td>
<td>0-108</td>
<td>2.0</td>
</tr>
</tbody>
</table>
Figure 4.2: Evolution of Maximum Courant number (CFL-number) in the domain of a characteristic run of LES-CMC.

Figure 4.3: Interaction of the CFD and the CMC-solver.
Chapter 5

Results and Discussion

The main objective of the project is to simulate a Spray A split injection setup. Firstly, the non-reactive vapour penetration length is calibrated in LES. Afterwards, also the reactive mixture fraction penetration lengths are presented. As a next step, a CMC mesh sensitivity analysis is carried out for a single injection, since multiple injection computations are computationally expensive. After having a feasible setup for LES in combination with CMC, the full Spray A split injection is simulated for both diesel-like (900 K) and LTC-like (750 K) operating conditions. The results are then compared to experimental data from [55]. Additionally, the setup of Case 1 is simulated by means of the direct integration combustion model in order to compare different aspects of the combustion process and the computational cost with LES-CMC.

5.1 Non-Reactive Simulation of Vapour Penetration Length

In order to be capable of simulating reactive simulations, the non-reactive flow field has to be validated, i.e. the spray vapour has to be compared to the experiment without having any chemical reactions. The basic phenomena of diesel combustion are an evaporating fuel spray that mixes with the ambient air (physical process) prior to combustion (chemical process). In order to have combustion, the oxidizer and the fuel need to mix, therefore, the combustion is mixing controlled. Since the mixing is such an important process, which underlies the oxidation of the fuel, it has to be validated beforehand. This can be accomplished by comparing the experimental non-reacting vapour penetration length with the simulated fuel spray. In that way it can be assured that the evaporating fuel spray is located at the right axial position over time. Past research in the framework of diesel spray combustion (e.g. [13]) has shown that accurate predictions of a single injection are possible with the k-ε model, where the Reynolds-Averaged Navier-Stokes equations are used. However, remarkably different conditions are estimated in a split injection setup. Since the current setup considers a constant-volume combustion chamber with high-temperature and high-pressure conditions representative of engine conditions, the first injection meets inert, quiescent ambient condition. The second injection, however, mixes with a cooler, vaporized fuel-ambient-gas mixture, produced by the first injection and enters a "slipstream". This causes a higher rate of penetration for the second injection compared to the first one [55], which is visible from the steepness of the curves in figure 5.1. The slipstream effect means that rather than forming a stagnation plane at the tip of the spray, as it is the case for the first fuel spray, the second injection follows the fuel ahead which is already moving downstream. Therefore, the enhanced velocity and turbulence magnitude caused by the first injection are complex effects that are difficult to predict by the k-ε model which was seen in [63]. Therefore, the simulations were accomplished using the LES turbulence model which is capable of accurately predicting highly turbulent fields. Simulating an evaporating fuel spray means representing phenomena such as primary and secondary droplet break-ups by mathematical models. The commercial CFD-solver Star-CD provides many models that allow accurate simulations of multiphase flows. The general approach in this framework is of the Lagrangian/Eulerian kind. In the case of the split injection, the atomization (i.e. primary
break-up) was computed using the Reitz-Diwakar (R-D) model [50] and for the secondary break-up (i.e., droplet break-up and vaporization) the Kelvin-Helmholtz and Rayleigh-Taylor (KHRT) model [42] was used. The results of the non-reactive fuel vapour penetration length of LES in the 900 K ambient condition is illustrated in figure 5.1. The solid lines starting from time zero indicate the first injection, while the dashed lines show the second ones. The black lines show the experimental data in connection with the yellow and light blue background shadings which represent the standard deviations of first and second injection, respectively. Three simulations using identical setups (Reitz-Diwakar/KHRT) are drawn in coloured solid and dashed lines. Since LES computes one single realization of a spray and no ensemble-average like RANS, the different runs show shot-to-shot fluctuations, i.e., the vapour penetration lengths are different for each run. The numerical results accurately predict the spray tip penetration lengths of both first and second injection. It has to be noted that the LES is capable of predicting the slipstream effect produced by the first injection including the created recirculation zone which enhances the penetration of the second injection.

The 750 K ambient condition cannot be validated since there are no experimental data. However, since in LES the large scales are resolved explicitly, the validity of the model is also assumed to hold in this case. Moreover, the ambient density is the same as in the 900 K case, so the spray will show the same behaviour.

5.2 Reactive Simulation of Vapour Penetration Length

From [55] it is known that the penetration of the reacting double injection into a 900 K ambient gas increases compared to the non-reactive case. The first injection penetrates faster due to thermal expansion which is triggered by chemical reactions. After the end of the first injection, the lifted flame advances from its lift-off length to the near-injector region which has been referred to as "combustion recession" [29]. Therefore, higher temperature, and thus lower density, can be estimated near the nozzle before the second injection starts, because high-temperature combustion for the first injection has occurred. Knowing that because of combustion recession the density in
the near injector region is reduced, it gets clear that the faster penetration of the second injection is beyond the effect of slipstream alone.

In figure 5.2 the black line with dots represents the reactive penetration length of the experiment of the first injection. Data about the penetration length of the reactive second injection is unknown up to the issuing of this report. The coloured, solid lines illustrate the five simulated reactive penetration lengths of the mixture fraction, where identical settings have been used. Like in the non-reactive case, shot-to-shot fluctuations are visible. It has to be noted, that the LES turbulence model is also capable of accurately predicting the reactive penetration length of the fuel spray, and accounts for thermal expansion throughout combustion. Due to the lack of information for the second injection, the validity is extrapolated from the non-reactive to the reactive case.

Considering the 750 K ambient temperature condition, similar assumptions as in the non-reactive case were made. However, it is known that for the case of 750 K, the reacting penetration length of the double injection is identical to that of the non-reacting case [55]. At the lower temperature, the first injection only undergoes high-temperature ignition at later timings and at a greater axial distance from the injector nozzle. Moreover, as there is no combustion recession in this condition, there are also no high-temperature zones near the injector orifice.

![Figure 5.2: Comparison of the reactive mixture fraction penetration length of LES to experimental data from [55]. Black line with dots: experimental, coloured lines: 5 different simulation realizations. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_2$.](image)

5.3 CMC Grid Sensitivity Analysis

Since there is no evidence in literature about what is the most suitable mesh resolution in terms of CMC for multiple injections in diesel spray combustion, a mesh sensitivity analysis is carried out. In the only case of numerical simulation of diesel spray combustion with LES-CMC [7], a one-dimensional CMC grid was applied. Other work, concerning lifted flames (partially premixed jets, e.g. methane/air or hydrogen/air) [37, 38], investigates how the dimensionality of the CMC implementation affects the solution. It has been shown that at stationary or quasi-stationary conditions, a flame can be well predicted by either a one or two-dimensional CMC grid. However, if this was also valid for a highly transient process, like it is the case in the split injection setup,
needs to be reassessed. Therefore, three types of CMC discretizations are tested: 1) The first method assumes negligible variation of conditional moments in radial direction, they only vary in axial direction and time, and is therefore termed "1D-CMC" [37]. 2) The second method allows variation of conditional moments in radial direction, but assumes still negligible variation in circumferential direction and is called "2D-CMCoarse". 3) The same assumptions apply as in 2), the only change is an increased CMC grid refinement in radial direction and is referred to as "2D-CMCFine". The ratio of LES to CMC cells is primarily limited by the computer resources. The smaller the CMC cell is, the less CFD cells are contained and stronger fluctuations of the scalar dissipation rate can be accounted for. Therefore, stronger turbulence-chemistry interaction can be captured and CMC predictions are likely to be more accurate [37]. However, using a very fine grid (e.g. 1 CFD/CMC cell) leads to a drastic increase in computational cost and to vanishing advantages of the LES-CMC compared to direct integration. In lifted flames, strong axial variations of the conditional moments are expected in the lifted flame and the ratio of 2 CFD cells for every CMC cell was chosen for the axial direction [37] and is constant for all the three CMC discretization options. Since the radial variations of the conditional moments are expected to be smaller, a ratio of 8 CFD cells for every CMC cell has been chosen for the "2D-CMCoarse" grid and a ratio of 4 for the "2D-CMCFine" grid. It is important to note that the grids are only refined in areas where the spray is expected, i.e. the nodes in axial z-direction are clustered around the area 0 to 60 mm and the nodes in radial r-direction are clustered around 0 to 10 mm. The fuel spray was not seen to exceed these dimensions in the experiment during the time of interest and therefore, also no combustion or variation of conditional moments is taking place in the mentioned zones. Like it was already noted, the eta-space is divided in 101 nodes clustered around the stoichiometric mixture fraction. Detailed information about the different grids can be taken from table 5.1.

Table 5.1: CMC grids used. \( N_r \) denotes the amount of CMC-nodes in radial and \( N_z \) the amount of CMC-nodes in axial direction. \( \Delta_{CMC}/\Delta_{LES} \) represents the size ratio of CMC to LES cells. \( \eta \) are the nodes in mixture fraction space.

<table>
<thead>
<tr>
<th>CMC Method</th>
<th>( N_r \times N_z = N_{tot} )</th>
<th>( \Delta_{CMC}/\Delta_{LES} (r) )</th>
<th>( \Delta_{CMC}/\Delta_{LES} (\eta) )</th>
<th>( N_\eta )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1D-CMC</td>
<td>( 1 \times 202 = 202 )</td>
<td>( \infty )</td>
<td>2</td>
<td>101</td>
</tr>
<tr>
<td>2D-CMCoarse</td>
<td>( 7 \times 202 = 1414 )</td>
<td>8</td>
<td>2</td>
<td>101</td>
</tr>
<tr>
<td>2D-CMCFine</td>
<td>( 12 \times 202 = 2424 )</td>
<td>4</td>
<td>2</td>
<td>101</td>
</tr>
</tbody>
</table>

5.3.1 Ignition behaviour

A critical event in diesel combustion is the ignition process. A first insight into the behaviour can be observed by investigating how and where the ignition takes place. First of all, the ignition delay (ID) from the simulation needs to be evaluated (\( \tau_{ID} \)), which is defined as the time from the start of injection (SOI) to the time where the maximum rate of maximum temperature in the domain occurs [44, 45]. Note that the maximum temperature is computed in each CFD cell (i.e. \( T_{\text{max}} = \max(T(x, y, z, t)) \)) and is therefore a very local event. The formal definition of the ignition delay is:

\[
\tau_{ID} = \tau \left( \max\left( \frac{dT_{\text{max}}}{dt} \right) \right) - \tau_{SOI}
\]  

(5.1)

The evolution of the maximum temperature of the three different CMC setups is visible in figure 5.3, where a single injection (half of the split injection) was performed. The experimental ID from [55] is \( \tau_{ID,exp} = 0.35 \pm 0.01 \) ms, which was found by high-speed schlieren imaging. The ID of the 1D-CMC simulation is 0.392 ms and is too long, whereas the 2D-CMCoarse simulation reaches a more accurate result of 0.359 ms, which is already in the standard deviation of the experiment. However, the most accurate computation of the ignition delay is accomplished by the discretization option 2D-CMCFine, which is 0.352 ms and corresponds perfectly to the experimental data. It has
to be noted that the skeletal mechanism for n-dodecane of Yao et al. [62] was particularly tuned for Spray A. In figure 5.3 it is clearly seen that once high-temperature ignition has occurred, the maximum temperature is nearly the same for the three types of CMC grids. However, the transient process of first-stage ignition is varying dependent on the CMC grid. First-stage (low-temperature or cool-flame) ignition can be defined as events where the temperature rise is less than 400 K above the ambient temperature [45], which is indicated by the orange dashed line. The flame produced by the 1D-CMC grid undergoes a late transition from first to second-stage ignition compared to the two-dimensional setups. The 2D-CMCcoarse setup shows an early and rapid transition followed by a small deceleration, whereas the 2D-CMCfine exhibits smooth transition to a high extent. The jump in maximum temperature is approximately 1320 K. From the point of view of the ignition delay, either of the two 2D-CMC grids can be chosen.

### Figure 5.3: Time evolution of the maximum temperature of Case 1. Compared are the three types of CMC grids. The dashed line is the single injection profile.

Until now, only non-dimensional analysis has been carried out looking at the maximum temperature. To have better insight into the problem, two-dimensional contour plots of the three types of CMC-discretizations are investigated at the individual time of ignition, where the closest time step of CFD-output compared the actual ID was chosen. As a very important specie generated during first-stage ignition [43], formaldehyde (CH$_2$O) is illustrated on the three plots on the left hand side in figure 5.4, whereas temperature is shown on the right hand side. Skeen et al. [54] showed that low-temperature chemical reactions initiate at the sides slightly behind the penetrating jet head and high-temperature ignition is known to proceed as a volumetric event, located at the spray head (i.e. a large volume of intermediates and radicals are consumed nearly simultaneously). It gets clear that the 1D-CMC fully fails to ignite at the tip, which is staying cold, and only shows high-temperature combustion at the sides. It is noted that radial convective and diffusive flux do not occur in 1D-CMC computations [38].

The contour plot computed by the 2D-CMCcoarse grid shows high temperature zones at the sides of the tip. In the colder core it is visible however, that CH$_2$O penetrates too far downstream, i.e. does not undergo transition into high temperature products in the tip area. This is physically questionable since the low-temperature products at the spray tip should give way to a large high-temperature combustion zone. Finally, the 2D-CMCfine discretization exhibits a high formaldehyde concentration only up to an axial distance of 22 mm. After that, second-stage ignition takes place in a more or less large volumetric zone, where formaldehyde gets consumed. This leads to the
5.3. CMC Grid Sensitivity Analysis

Figure 5.4: Contour plots at the individual time of high-temperature ignition. The solid white line represents the stoichiometric mixture fraction. Comparison of three types of CMC discretizations: 1D-CMC, 2D-CMCcoarse and 2D-CMCfine. Left side: formaldehyde (CH₂O), right side: temperature. Ambient conditions: 900 K, 22.8 kg/m³, 15 % O₂.

Conclusion that the 2D-CMCfine grid can capture the highly transient ignition process in the most accurate way.

5.3.2 Flame Structure Development

The flame structure is again analysed at later stages. The time step 0.7 ms was considered to give fair insight into the intermediate flame development, because it is approximately in the middle between ignition and 1.0 ms (which is the end of the considered time frame for the sensitivity analysis). In figure 5.5 on the top right hand side, it is visible that the 1D-CMC still did not succeed to ignite at the spray head, in fact it stays cold (i.e. 900 - 1000 K) despite the fact that this should be the main spot of high-temperature ignition. Another problematic observation is that there is, considering the temperature plot, an unrealistic "cut-off" of high temperature at an axial location of 9 mm distance from the injector orifice although stoichiometric fuel/air mixture is available. This trend is again discussed later.

For the two-dimensional cases, the soot precursor specie acetylene (C₂H₂) is considered. For both 2D-CMCcoarse and 2D-CMCfine, the main soot cloud is located in the rich zone of the spray head, which is reasonable. Additionally, both discretization options exhibit high soot concentrations at lateral locations of the spray. The 2D-CMCcoarse case, however, appears to have a low (YC₂H₂=0.0075, green) soot concentration core between 15 and 32 mm, which is also visible as a mid-temperature (T=1500 K) zone. It appears as if the CMC cells located on the z-axis lacked to proceed to second-stage ignition, which is a questionable trend. Considering the computation by the 2D-CMCfine grid, the soot cloud is distributed more or less evenly and does not show any non-igniting cells.

Moreover, the mentioned time step is appropriate to show the transition of conditional temperature starting upstream (in the near-nozzle area) from a non-burning to a rigorously burning mixture. At 0.7 ms ASOI, convection and diffusion effects start to dominate, and energy is transported against the flow direction, i.e. combustion recession is likely to commence since the injection has...
already terminated (at 0.5 ms ASOI). To investigate this behaviour, the axial distribution of the mean conditional temperature at $\eta = 0.0463$ is shown in figure 5.6. The one-dimensional CMC case shows a steep increase of temperature and fluctuations hardly exist. This is in accordance to what was seen in [37]. Rather than a transition, there is a cut-off in temperature, like it was mentioned before. For both 2D-CMC cases, the transition is not as abrupt and large fluctuations in the order of 200 - 300 K are observed at the flame base. These fluctuations are likely to be caused by the interaction between radial and axial transport of the conditional moments into the CMC cell [37]. Moreover, since the CMC cells are much smaller from 1D compared to 2D-CMC, the mixture fraction contains very localized information whose time history influences the conditional moment additionally. In LES-CMC, the location of the minimum distance between nozzle exit and flame base varies in every spatial direction and time, and the flame elements that form the flame base might be ignited by radial transport of energy and mass [38]. Since this transport is lacking in the one-dimensional CMC calculation and localized information is not captured, the flame base could have difficulties to ignite [37]. As it was seen before, the 1D-CMC simulation shows a cold spray head also in terms of conditional temperature.

Comparing the two 2D-CMC cases, it gets clear that both show a transition with large instantaneous fluctuations from the cold flame base to the lifted flame. Noteworthy is that the 2D-CMCfine computation shows an earlier combustion recession, i.e. there are hotter zones at low axial distances from the injector. This could be due to the enhanced radial transport, since it is more refined. From this point of view it can be concluded, that a 1D-CMC calculation is insufficient for diesel sprays and two-dimensional models are able to realistically capture the conditional temperature.

Having already considered the ignition time and 0.7 ms ASOI, 1.0 ms is again analysed. The three CMC discretizations are compared to each other in figure 5.7. The one-dimensional method succeeded to burn in the near-injector area and combustion recession is visible, there is no cut-off in temperature anymore. However, it still failed to ignite at the tip. Furthermore, the tip of the 1D-CMC case is seen to travel further than the 2D-CMC cases. In [38] it is stated that stationary or quasi-steady state conditions can be predicted well for all (1D and 2D) configurations, however
5.3. CMC Grid Sensitivity Analysis

since this setup only considers transient processes, this does not apply for the 1D-CMC setup.
Comparing the temperature plots of both two-dimensional cases in figure 5.7, there are hardly any
differences visible neglecting the shot-to-shot variability. This supports the hypothesis that once
the transient ignition process is over and a broad high-temperature flame is established, the radial
grid resolution of CMC does not have a very high influence. However, the 2D-CMCfine simulation
shows a broader, more concentrated soot cloud in the rich core of the spray head than the 2D-
CMCcoarse does. From Pei et al. [45] it was seen that the finer CFD-meshes produced a higher
magnitude of soot (measured by YC_2H_2) and the soot cloud appeared to be more spread out than
less resolved cases. Since in [45] a δ-function combustion model was implemented, the combustion
model is solely dependent on the CFD-mesh resolution. It is believed that similar effects can be
achieved with a CMC-grid refinement (2D-CMCfine).

5.3.3 Thermal Expansion

Another characteristic measure of the quality of the burning process is the thermal expansion. It
happens as soon as the temperature rises and as a consequence, the density drops which leads to
expansion of the burning gases. As a simple first measure, one can start from the ideal gas law:

\[ \rho R T = p \]  

(5.2)

where \( \rho \) is the density, \( R \) the specific gas constant, \( T \) the temperature and \( p \) the pressure. Recalling
that a small stoichiometric portion of mixture is ready to burn before ignition, we assume there
are two states: the un-burnt (u) and the burnt (b) mixture. Therefore we can write:

\[ \frac{\rho_u}{\rho_b} = \frac{T_b}{T_u} \frac{R_b}{R_u} \frac{\rho_u}{\rho_b} \]  

(5.3)

Neglecting the change of the specific gas constant and assuming a constant pressure in that instant,
we can estimate the ratio of density by the ratio of burnt to un-burnt temperature: \( \rho_u/\rho_b = T_b/T_u = 2300/900 \approx 2.5 \). Therefore, the specific volume rises by a factor of 2.5. Since we are in
non-premixed combustion, this estimation only holds for a small control volume where fuel and air
is premixed and for a very short time period.

The thermal expansion is considered in figure 5.8, where the left column illustrates the non-reactive
contour plots of the fuel vapour, the middle and right column show the reactive 2D-CMCfine and
Chapter 5. Results and Discussion

Figure 5.7: Contour plots at time equal to 1.0 ms. The solid white line represents the stoichiometric mixture fraction. Comparison of three types of CMC discretizations: 1D-CMC, 2D-CMCcoarse and 2D-CMCfine. Left side: acetylene ($\text{C}_2\text{H}_2$), right side: temperature. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_2$.

1D-CMC simulation, respectively. The time steps are chosen to be right after ignition (0.4 ms) and two later time steps, where combustion is progressing. Initially, in both reactive cases, nearly no thermal expansion is visible, since high temperature combustion just has started. At 0.6 ms, the fuel spray is already slightly spread out, mostly in axial direction. The difference between the one and two-dimensional case is negligible. At 0.8 ms, the expansion (which can also be seen by the increasing distance between the spray border line and the stoichiometric line) of the 1D-CMC takes still place predominantly in axial direction, the radial growth is observed only marginally. The two-dimensional CMC calculation exhibits both radial and axial expansion which is most likely caused by the radial transport of the conditional moments. The 2D-CMCcoarse was seen to produce very similar results to the ones from the 2D-CMCfine case. From the spray physics point of view, it makes more sense that the spray expands both axially and radially after combustion. Therefore, 2D-CMC is the better option.

5.3.4 Evolution of Temperature Conditional on Mixture Fraction

After studying the transient process in a spatial manner, the temporal evolution of scatter plot of temperature in mixture fraction space is examined in figures 5.9 - 5.11, to further understand the ignition process. Around 0.125 ms, first-stage ignition is initiated in a very lean mixture (leaner than $\xi_{st} = 0.0463$) and propagates into rich mixtures (richer than $\xi_{st}$) at later stages. This observation of initiation of first-stage ignition under fuel-lean conditions was also seen by [45, 54] in a numerical and experimental manner, respectively. The lean mixture ignition might be caused by higher local temperatures of the ambient gas, with later propagation to low temperature reactions in the rich mixtures due to convective and diffusive transport of products from lean combustion into rich zones [45]. At 0.2 ms, different levels of progress of first-stage ignition are visible, where the higher temperature cells appear in a rich mixture, some zones in the 2D-CMCfine case are close to 1200 K. Having first-stage ignition or low temperature combustion (defined as temperatures below 1300 K for this case), around 0.3 ms the 1D-CMC has not yet progressed to high temperature combustion, whereas the two-dimensional CMC cases did. As it was already
stated, main ignition happens between 0.35 and 0.4 ms for all three cases. From figures 5.9 -
5.11 it can be seen that the second-stage ignition events are happening in slightly rich zones
and propagating towards stoichiometry later. At 0.4 ms there is almost no difference besides the
maximum temperature. For 0.7 ms and 1.0 ms it is visible that the 1D-CMC discretization is
not able to have high temperature combustion for all the CFD-cells containing fuel (we recall
the non-igniting tip). The 2D-CMC coarse grid is capable of having mostly high temperatures for
fuel/air mixtures around stoichiometry. However, the computation using the 2D-CMC fine grid
exhibits the fastest transition from low to high temperatures, especially seen at 1.0 ms. The
peak temperatures is seen, as expected, around the stoichiometric mixture fraction, whereas the
maximum temperature decreases towards rich and also lean mixtures [45]. It can be concluded
that both 2D-CMC grids produce reasonable temperature distributions over time. A difference is
that the finer grid shows a faster transition to high-temperature combustion, meaning that it burns
more rigorously (especially seen at 1.0 ms). After these considerations, it is further recommended
to use a 2D-CMC discretization.

Figure 5.8: Comparison of the thermal expansion between the non-reactive and the reactive case.
The solid thin white line represents the stoichiometric mixture fraction and the dotted white line
shows the spray border ($\xi = 0.01$) and the solid thick magenta lines represent the spray border of
the non-reacting case at the same instant of time.

Figure 5.9: Evolution in time of temperature conditional on mixture fraction for the whole computa-
tional domain of the 1D-CMC computation. The black dashed-dotted line indicates $\xi_{st}$. 
Figure 5.10: Evolution in time of temperature conditional on mixture fraction for the whole computational domain of the 2D-CMC coarse computation. The black dashed-dotted line indicates $\xi_{st}$.

Figure 5.11: Evolution in time of temperature conditional on mixture fraction for the whole computational domain of the 2D-CMC fine computation. The black dashed-dotted line indicates $\xi_{st}$.

5.3.5 Pressure Rise

A comparison of the pressure rise is seen in figure 5.12. Since the pressure rise rate scales with the apparent heat release rate (AHRR), the simulated pressure rise ($p(t) - p_0$) is taken as a qualitative indicator of combustion, i.e. $\frac{dp}{dt} \sim$ AHRR. The pressure starts to rise significantly after 0.3 ms for all three CMC types. In agreement to what was seen from the scatter plots, the one-dimensional CMC type is reluctant concerning transition to high temperature combustion which is also visible at the pressure rise. Recalling the maximum temperature plot (figure 5.3) it was seen that the coarser CMC grid showed an earlier rise in maximum temperature, which might also be the cause of an earlier pressure rise compared to the finer grid (comparing the blue to the red solid line). Nevertheless, after 1.0 ms the 2D-CMC fine case shows approximately the same magnitude of pressure rise. The difference of the transition of the blue and red curve regarding pressure rise could also be a shot-to-shot fluctuation.
5.3. CMC Grid Sensitivity Analysis

Figure 5.12: Pressure rise of LES-CMC, comparison of different CMC discretizations. The dashed line shows the single injection profile.

5.3.6 Computational Cost

Table 5.2 shows that the computation is not only dependent on the CFD mesh (which was the same for all three cases) but also the CMC grid. The 2D-CMCcoarse is roughly 60 % more expensive than the one-dimensional case, having a factor of 7 times more CMC nodes and the 2D-CMCfine discretization takes up twice as much CPU time, using twelve times more CMC nodes. However, recalling the benefits induced by the fine CMC resolution, the higher cost is justified and is worthwhile spending, since the LES-CMC approach considers very local and transient effects. For the upcoming split-injection setup with two subsequent injections it is recommended to account for a very detailed interaction of the two sprays.

Table 5.2: Computational cost of different CMC types for a single injection (0.5 ms).

<table>
<thead>
<tr>
<th></th>
<th>1D-CMC</th>
<th>2D-CMCcoarse</th>
<th>2D-CMCfine</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of CMC nodes</td>
<td>$1 \times 202 = 202$</td>
<td>$7 \times 202 = 1414$</td>
<td>$12 \times 202 = 2424$</td>
</tr>
<tr>
<td>1 ms total CPU time [h]</td>
<td>47.0</td>
<td>50.2</td>
<td>47.5</td>
</tr>
<tr>
<td>Number of processors*</td>
<td>48</td>
<td>72</td>
<td>96</td>
</tr>
<tr>
<td>Total hours/proc. [h]</td>
<td><strong>2254.5</strong></td>
<td><strong>3616.5</strong></td>
<td><strong>4562.7</strong></td>
</tr>
<tr>
<td>Ratio</td>
<td>100 %</td>
<td>160.4 %</td>
<td>202.4 %</td>
</tr>
</tbody>
</table>

*on EULER-cluster

5.3.7 Summary of the Grid Sensitivity Analysis

Considered were three types of CMC discretization, having a one-dimensional, a coarse and a fine two-dimensional CMC grid. The ignition delays were computed and compared to the nominal value and determined to have $+12 \%$, $+2.6 \%$ and $+0.6 \%$ deviation for the 1D, 2Dcoarse and 2Dfine case, respectively. The contour plots of formaldehyde and temperature during ignition showed further that the distribution is physically the most realistic for the fine 2D-CMC grid. Also during transition from low to high temperature combustion around 0.7 ms, the soot precursor computation was evenly distributed, whereas in the other two cases questionable patterns were visible. The conditional mean temperature of 1D-CMC at 0.7 ms step showed a physically wrong
cut-off (i.e. the temperature is jumping from low to high temperature from one CMC cell to the next), whereas both two-dimensional cases exhibited a transition with instantaneous large scale fluctuations which was also seen in literature [37]. Comparing the cases at 1.0 ms, the contour plots of the fine resolved CMC grid showed the most spread distribution and the highest amount of the soot precursor in the spray head which is known to be most accurate (seen e.g. in [45]). Furthermore, the thermal expansion was considered. From the spray physics point of view, it makes more sense that the spray expands both axially and radially after combustion and therefore, 2D-CMC is the better option. Analysis of the scatter plots of temperature showed that ignition is initiated in lean mixture areas, propagates to rich mixture zones undergoing low temperature combustion and travels back close to stoichiometry, where high temperature combustion occurs. This pattern was seen in all of the CMC types. However, the fastest transition from low to high temperature combustion was seen by the fine 2D-CMC type. The quantitative pressure rise showed no evidence for choosing the fine over the coarse CMC resolution. In conclusion, the 2D-CMC fine grid is obviously the most expensive choice (double the cost of 1D-CMC) but is able to correctly compute qualitative CH$_2$O and C$_2$H$_2$ spatial distributions, transition from low to high temperature ignition and therefore, it is the best variant, since the simulation should be as predictive as possible.
5.4 Case 1 (900 K): Reactive Simulation Analysis of Split Injection

Case 1 considers the split injection setup of an \( n \)-dodecane injection into 900 K ambient gas, detailed setup information can be found in chapter 3. This case resembles the diesel-like operating condition, where multiple injections offer increased flexibility in terms of heat-release timing, which can improve fuel economy as well as the possibility to lower \( \text{NO}_x \)/soot emissions. After different considerations in the sensitivity analysis, the 2D-CMCfine grid is used for the further study. In total, five realizations of this setup with identical initial conditions were carried out for ensemble averaging. First of all it is investigated how the second injection event is computed in terms of conditional moments. As a second step, the direct comparison of the simulation to the experiment follows.

5.4.1 Analysis of First Injection

The flamelet analysis is similar to the one seen in figures 5.9-5.11, but instead of analysing the whole CFD-domain, only one CMC cell is considered. The CMC model arose from the laminar flamelet model (which was derived in [46]), in contrast to the flamelet model it considers a flamelet in every CMC cell. A characteristic CMC cell has been chosen at the coordinates \( x = 1 \) mm and \( z = 22 \) mm to show the evolution of the conditional temperature for the first injection in order to compare it later to the one from the second injection. The black line is the adiabatic mixing line of fuel and ambient oxidizer and is still the predominant state at 0.2 ms ASOI. The blue line shows first-stage ignition in a rich mixture which is advancing rapidly towards second-stage ignition seen by the brown curve. The rest of the coloured lines shows the transition to high temperatures including propagation of the peak towards stoichiometry, like it was seen in the scatter plots of the sensitivity analysis.

![Figure 5.13: Characteristic temperature profile evolution in mixture fraction space for the first injection.](image)

5.4.2 Analysis of Second Injection with Reinitialization

In the above-mentioned sensitivity analysis, only the first injection was considered. However, the split injection contains two fuel sprays, where the second injection is modelled by the CMC multiple injection approach described in section 2.4. We recall that transport equations for the conditional moments (CMC equations) are solved temporally (constant time step) and spatially (on each CMC node). Moreover the conditional species and temperature profiles are formed in an additional dimension, the \( \eta \)-space (\( \eta \) is the sample space variable of the mixture fraction \( \xi \)). Therefore, the species and temperature are conditioned on the total mixture fraction, which is \( \text{MF}1 \) until 1.0 ms and the start of the second injection. After the second injection has started, the CMC equations are conditioned on the total mixture fraction (\( \text{MF}1+\text{MF}2 \)) and a reinitialization...
is necessary in order to prevent the second injection from instant ignition. As soon as a certain quantity of MF2 enters a CMC cell, the temperature and species profiles are reinitialized according the model described earlier. In the following, the conditionally filtered quantities are considered, however for the ease of comprehension they are simply called conditional species and temperature. In the following, three locations of CMC cells are considered, which contain different amounts of initial MF1 and temperature. The correspondent mixture fraction and temperature distribution can be found in the contour plots of figure 5.17.

**Reinitialization at Lean Conditions**

A characteristic reinitialization of the conditional species, such as acetylene (soot precursor), formaldehyde (low-temperature combustion indicator) and oxygen, as well as the conditional temperature, is illustrated in figure 5.14 for a CMC cell having a lean distribution of MF1.

![Temperature profile evolution in total mixture fraction space](image1)

![C\textsubscript{2}H\textsubscript{2} profile evolution in total mixture fraction space](image2)

![Oxygen profile evolution in total mixture fraction space](image3)

![CH\textsubscript{2}O profile evolution in total mixture fraction space](image4)

Figure 5.14: Temperature, acetylene, oxygen and formaldehyde evolution in total mixture fraction space (MFT) for a lean initial MF1 distribution, before and after reinitialization. Location of the CMC-node: $x = 1$ mm and $z = 4$ mm, outside of the liquid fuel core.

The conditional species and temperature profile before reinitialization are illustrated by the black solid lines (i.e. before a CMC cell senses the new fuel coming from MF2), whereas the reinitialized profiles are depicted as the dark blue solid lines. After that, the evolution in time is shown by the other coloured lines. The profiles are reinitialized 37.5 $\mu$s after the second injection starts, because the CMC cell has an axial and lateral off-set (located at the coordinates $x = 1$ mm and $z = 4$ mm) to the injector. The ignition of the second injection happens similarly to a single injection seen in figure 5.13. However, in figure 5.14 a), one can clearly see that the first-stage ignition occurs
in a more rich mixture area than the ignition of the first injection, and is propagating towards stoichiometry (dashed-dotted line). About 0.16 ms after the second injection, the conditional profile associated to the second injection reaches a similar profile (red curve) as the first injection prior the second injection. However, since only one single CMC cell is considered, the ignition delay of the second injection cannot be determined and is going to be described later.

The evolution of the conditional oxygen profiles (figure 5.14 c)) show a similar behaviour, however the distribution of the red line indicates that the ignition is only locally at stoichiometry since there is a probability of oxygen in richer parts of the mixture fraction space.

The reinitialization process of the soot precursor (figure 5.14 b)) shows that after reinitialization there is almost no probability of having acetylene, which is physically realistic since the new fuel stream is still cold and needs to ignite prior to soot development. The light blue solid line indicates that after 0.2 ms after the second injection, the species profile has a similar state to the one before the second injection, having a much bigger spread than before second injection though.

Analysing figure 5.14 d), one can notice looking that the second profile after reinitialization (orange solid line), that the peak mass fraction is already considerably high (i.e. \( \sim 50\% \) of the peak value of the black line). This indicates that first-stage ignition is promoted rapidly (about 0.04 ms after reinitialization) which could be caused by the employed chemical mechanism. About 0.11 ms after reinitialization (green line) the value has reached a similar concentration as before reinitialization, with a decreasing tendency.

**Reinitialization at Stoichiometric to Rich Conditions**

Reinitialization of the conditional species and temperature profiles located at \( x = 0.5 \text{ mm} \) and \( z = 4 \text{ mm} \) showed a different behaviour, which is seen in figure 5.15. The black line shows the temperature and species profiles before reinitialization and the coloured lines represent the states afterwards. The temperature profiles (figure 5.15 a)) did not exhibit a major difference if the states before and after reinitialization are compared. However, the pink line represents the temperature profile after reinitialization and one has to note that the left part of the profile is retained, therefore it has to be assumed that the MF1 conditions were stoichiometric to rich before new fuel was entering a cell. At the next considered time step (blue line), the temperature already advanced to a similar profile as seen before reinitialization, therefore it burns immediately.

Considering the evolution of the soot precursor in figure 5.15 b), these findings are strengthened. The pink line is again the reinitialized profile, where \( \text{C}_2\text{H}_2 \) mass fractions in the order of 0.006 are prevailing. Second-stage ignition happens within approximately 60 \( \mu \text{s} \) at the time when the brown line is established. At this time step, a similar maximum concentration is reached as before reinitialization. Therefore, it is expected that high temperature combustion species are being produced very rapidly.

In figure 5.15 c) the mentioned effects are also visible. It is noticed that the oxygen concentration is increased only for a very short moment, afterwards second-stage ignition is already promoted which leads to fast consumption of \( \text{O}_2 \). However, the increased probability of oxygen in richer regions prevails to a certain extent.

The formaldehyde profiles seen in figure 5.15 d) show that first-stage ignition is nearly instantaneous after reinitialization (pink profile). At later time steps, the probability is shifted towards richer regions of the total mixture fraction and is low at stoichiometry.

In figure 5.17, the initial conditions of the MF1 distribution are mostly lean or close to stoichiometry. Any addition of fuel from the second injection leads to a shift to richer conditions, which are, given also the high temperatures, prone to ignite immediately. It is expected that for this initial state of mixture fraction, the conditional profiles are reinitialized at an instant and are catapulted to high temperature combustion again. The fast transition could be due to the chemical mechanism or due to a lack of accuracy in the reinitialization model. The fast transition will lead to high temperature combustion products near the nozzle, which might be questionable. Since LES-CMC computes very local, instantaneous quantities, the reinitialization model might be overstrained by high frequent fluctuations. Nevertheless, aforementioned findings only consider one CMC-node. It is expected that the general accuracy is granted to predict the combustion of a second injection.
Figure 5.15: Temperature, acetylene, oxygen and formaldehyde evolution in total mixture fraction space (MFT) for a stoichiometric to rich initial MF1 distribution, before and after reinitialization. Location of the CMC-node: $x = 0.5$ mm and $z = 4$ mm.

Reinitialization of Only Fuel-Rich Conditions

At the same axial distance as before, but in the centre axis (at the location $x = 0$ mm and $z = 4$ mm), the reinitialization of temperature and species profile looks different and is illustrated in figure 5.16. The reinitialization happens at approximately 1.04 ms ASOI like the two cases before, although it is not shown here. The black lines show the temperature and species profile before reinitialization, whereas the coloured lines represent the profiles after reinitialization. The lowering of the temperature and combustion species (figures 5.16 a)/b)/d)) is achieved through the adiabatic mixing of the new, rich and cold MF2 with the old, lean and hot MF1. The flame is extinguished at this point, therefore the oxygen mass fraction seen in figure 5.16 c) is increased to ambient conditions and the adiabatic mixing line is established. Despite the propagation of the conditional profiles towards a burning solution begins to show, an eventual stagnation is seen (not shown here). Since the mentioned node is located right above the nozzle, liquid fuel is transported to this specific CMC cell which prevents it from burning, as long as the injection is not terminated. The evolution of the flamelet seen in this CMC cell is predominantly influenced by convection effects.
5.4. Case 1 (900 K): Reactive Simulation Analysis of Split Injection

Figure 5.16: Temperature, acetylene, oxygen and formaldehyde evolution in total mixture fraction space (MFT) for an only fuel-rich MF1 distribution, before and after reinitialization. Location of the CMC-node: $x = 0$ mm and $z = 4$ mm, inside of the liquid fuel core.

Mixing and Combustion of the Second Injection

Figure 5.17 shows the contour plots of mixture fraction and temperature after the start of the second injection. The white text in the plots shows the time. At 1.0 ms, the second injection is about to start and a mostly lean trail is left from the first injection. At 10 mm axial distance from the injector, a stoichiometric to rich zone is seen. The temperature around the nozzle is still medium high (~1500 K) due to combustion recession. The next time step (1.05 ms) shows that the second fuel spray penetrates into this medium hot field. The three different kinds of reinitialization, as it was shown before, are expected to take place, preventing the second injection from instant ignition. At 1.1 ms, the stoichiometric mixture fraction cloud from the first injection is already hit and mixes with the new fuel injection. This is represented by three small yellow to orange spots (slightly above 1700 K) located laterally and at the tip of the spray head. No significant differences are observed at 1.15 ms, whereas at 1.2 ms, high temperature combustion is spotted. At the sides of the second spray head, several spots with temperatures around 2000 K are formed.

Considering the ignition delay definition from equation 5.1, this does not hold in this case. Since the maximum temperature is already high, the temperature gradient cannot be used for this calculation. The second injection clearly ignites earlier than the first injection, which is seen from the conditional profiles as well from the contour plots. Detailed insight of the complete split injection in terms of mixture fraction, temperature and the radical OH can be found in the appendix, figures A.1-A.3. Pressure rise and AHRR might give more insight into this topic, but are considered later.
Summary of Second Injection

Two different aspects of simulating subsequent injections have been considered, namely the reinitialization of the conditional profiles and the time evolution of contour plots from mixture fraction and temperature. The reinitialization process is strongly dependent on the initial MF1 distribution in a CMC cell before new fuel (i.e. second injection) enters the domain. Therefore, three different reinitialization types where characterised, reinitialization under lean conditions, stoichiometric under lean conditions, stoichiometric to rich conditions and at only fuel-rich conditions. The first and the latter type appear to prevent the injection from immediate ignition. The second type, however, promotes high temperature combustion very rapidly, because the initial mixture fraction distribution is at lean and close to stoichiometric conditions, so the second injection pushes it towards slightly fuel-rich conditions, which leads to ignition. In LES, the computation of very local quantities and fluctuations is possible which influences also the reinitialization process. Therefore, if a cell still contains combustible mixture before new fuel arrives, it will continue burning even after mixing with the new fuel stream. The observed effects are estimated to be reasonable and the simulation of the split injection can be compared to the experiment as a next step.
5.5 Case 1 (900 K): Reactive Simulation and Comparison to the Experiment

A direct comparison of the experimental findings from [55] is considered. An ensemble average of five realizations was carried out, i.e. the exact same setup with identical initial conditions was simulated five times and then ensemble averaged. Since LES only computes a single realization and not an ensemble average like RANS, shot-to-shot fluctuations are expected. According to Pei et al. [45], a "relevance index" is introduced in order to estimate the number of LES realizations required to compare with experiments. In the mentioned study, averaging of 5 realizations produces a relevance index of about 99 % (i.e. similarity) for mixture fraction. Moreover, it was found that 6 realizations are enough for temperature, whereas 8 and 14 realizations are required for soot and OH, respectively. In the current study, five realizations are considered for the ensemble average to have 99 % similarity of the mixture fraction. Detailed contour plots of the split injection simulation can be found in the appendix A.

5.5.1 Pressure Rise

The black solid line in figure 5.18 shows pressure rise of the simulation and the black solid line with dots illustrates the experimental pressure rise. Like it was already seen, the ignition delay is predicted accurately. The total measured pressure rise in the experiment was approximately 25 kPa, whereas the simulation only predicted around 16.5 kPa, which is 34 % too low. A possible reason for the lack of correct prediction of the pressure rise could be a different total volume (caused by the injector, intake/exhaust valve, etc.), comparing the combustion vessel with the computational domain of the simulation. The qualitative pressure evolution seems to be accurate, however the quantitative prediction is questionable. A possible reason is that mixing of the turbulence model is underestimated. Tuning the correspondent constants could lead to higher pressure rise, since diesel combustion is mixing-controlled burning, however decrease also the penetration length. Moreover, the CMC model could be the issue. Further work is needed to overcome this discrepancy.

Figure 5.18: Ensemble average of the pressure rise of the split injection simulation using 2D-CMCfine (solid line) and the experiment (solid line with dots). The dashed line shows the injection rate. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_2$. 
5.5.2 Apparent Heat Release Rate

The black line with circles in figure 5.19 shows the experimental data, the red line illustrates a single realization and the blue line shows the ensemble average of the AHRR. The experiment shows large scale fluctuations during the ignition process (0.2 – 0.4 ms), whereas the simulation shows a more smoothed profile. The first peak in the experiment indicates first-stage ignition, which is also visible as a small bump of the blue line shortly before 0.2 ms. The second peak of the AHRR is formed due to second-stage ignition, which is not distinctly visible in the shape of the blue curve. After these two peaks, the experimental AHRR has a smooth shape with two clear maxima coming from the correspondent injections, which occur at 0.5 and 1.5 ms, respectively. The simulated heat release rate is delayed by approximately 0.1 ms, having the maxima around 0.6 and 1.6 ms. Concerning the AHRR-amplitude, the experimental maxima (of the smooth part) are approximately 63 and 69 J/ms, respectively, whereas the simulated average maxima were computed as approximately 46 J/ms. Additionally, the experimental AHRR shows values below zero, indicating heat losses, whereas the simulation was considered as adiabatic.

Furthermore, it is observed that the AHRR is decreasing at the time that the second injection starts. Therefore, the increase in AHRR is attributed to the combustion of the second injection and is utilized to indicate ignition. According to [55], the AHRR-based ignition delay time for the second injection is evaluated based on a 20 % rise in AHRR after the minimum near 1 ms (yellow circle in figure 5.19). The ignition delay was computed for every realization, resulting in the ensemble average of 0.15 ± 0.07 ms (90 % confidence interval). The experiment ignited at 0.17 ± 0.01 ms, so the result of the simulation is very accurate.

In conclusion, the simulation is able to capture the trends of the AHRR very well. Qualitative and quantitative computations need improvement, however. Qualitatively, the connection to the pressure rise is obvious. A possible measure to enhance the intensity of combustion would be to increase the mixing of oxidizer and fuel in order to accelerate the burning process.

5.5.3 Comparison of Density plots to Schlieren Images, Reactive Setup

Since the schlieren images show very instantaneous details, only one realization is shown in figure 5.20. However, each schlieren image is taken from a unique experiment under identical ambient and injection conditions, whereas the LES-CMC simulation shows one single run. The first and every other plot (in vertical direction) shows the experimental schlieren images, where the red lines indicate the location from the 355-nm PLIF signal, which are needed later. The second and
every other plot (in vertical direction) shows the density contour plots where the red lines indicate iso-contours of formaldehyde and acetylene.

The penetration length of the first injection is captured accurately throughout the whole simulation time, like it was reported before. The lateral expansion tends to be slightly under-predicted. The penetration length of the second spray head is not as well predicted as the first one, but still reasonable. The non-reactive vapour penetration length of figure 5.1 showed accurate results for the second injection. However, since the reactive penetration length study of section 5.2 only contains data from the first injection (other data is not available up to the date of writing), a different behaviour is possible for the reactive penetration length of the second injection. Around 1.2 ms ASOI, the prediction of the penetration length is the weakest, however, it appears to improve considerably towards later time steps. The lateral spreading of the second spray head is too narrow.

Figure 5.20: Time sequence of schlieren images compared with the computed contour plots of density, single realization. Order of the plots: first plot shows experimental results ($\mu$s in title) with direct comparison to the simulation (ms in title) arranged below. In the experimental images, the red lines indicate the location from the 355-nm PLIF signal. In the simulation plots, the red solid and black dotted lines show iso-contours of formaldehyde and acetylene ($YCH_2O + YC_2H_2 = 0.001$) and the spray border ($\xi = 0.01$), respectively. Experimental data from [55]. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_3$. 
The reason is either the thermal expansion, the atomization model of the CFD-solver or an under-resolved CFD-grid. During the project different settings for the R-D atomization were tested, such as nozzle contraction factor and discharge coefficient. Indeed, it led to the effect that the radial spreading of the spray was increased, however the penetration length of the spray decreased remarkably. From this point of view it was chosen to focus the efforts on achieving the correct penetration length rather than the radial spreading, because the comparison of the latter can only be done qualitatively (i.e. compare schlieren images to contour plots). A CFD cell size sensitivity analysis has not yet been done, however, Pei et al. [45] shows how a refined CFD grid spreads out the spray in radial direction.

To conclude, the qualitative comparison of the density contour plots with the schlieren images are generally satisfactory, however, show weaknesses in terms of radial spreading.

### 5.5.4 Comparison of C2H2 and CH2O to 355 nm PLIF

As a next step, the ignition and combustion process is qualitatively compared to the experiment, which is illustrated in figure 5.21. Note that the colour scale of the experiment and the simulation are not necessarily identical, they only allow for a qualitative comparison (this applies to all the PLIF plots in this report). Furthermore, the reader has to keep in mind that the colour scales of CH2O and C2H2 differ by a factor of 4 to make the different combustion phenomena more visible. The experiment, on the other hand, uses the same signal intensity for both CH2O and PAH. The first and every other plot shows a time sequence of PLIF images. Note again that formaldehyde PLIF only provides a single image per realization of an experiment. Therefore, each PLIF image is from a unique experiment. The second and every other plot shows the contour plots of CH2O in the lower half and of C2H2 in the upper half. CH2O is an indicator of low temperature combustion whereas C2H2 is a precursor of soot, which is formed in high temperature combustion. For the simulation, a considerable rise in YC2H2 from one axial location to the other is taken as the lift-off length.

Beginning at 0.7 ms ASOI, i.e. 0.2 ms after the end of the first injection, the experiment shows formaldehyde around the characteristic lift-off length of 16 mm. At farther axial locations (35-40 mm), a fluorescence signal from PAH is observed. For the first injection the distinction between PAH and formaldehyde is certain, since the signal differs in time, space and the signal intensity [54]. The simulation shows no clear distance at which all formaldehyde is consumed (that is why C2H2 is taken as a lift-off indicator), there is however a broader spatial distribution of CH2O in the area of the nozzle up until 18 mm, which does not appear as radially spread as the experiment. After this specific distance, it prevails in the thin rich core of the spray. This might be due to a lack of radial transport of heat towards the centre of the spray. The soot precursor shows a considerably high presence after approximately 22 mm, which is taken as the lift-off length and is therefore 6 mm too long.

Later at 1.0 ms, combustion recession occurred and all formaldehyde has been consumed near the lift-off length which is seen as a strongly reduced PLIF signal intensity. In contrast, the signal of the downstream PAH has broadened and intensified. These processes are also predicted by the simulation, CH2O in the upstream region is not observed and the soot cloud at the spray tip is predicted well, however the radial expansion is slightly too small.

The third image pair is recorded around 1.1 ms ASOI, where the liquid from the second injection is visible at a penetration length of about 13 mm. According to [55], it is injected into the remaining high temperature products including radical species of the combustion recession of the first injection, which are above 900 K. As a consequence of these high temperature products, a very rapid progression into second-stage ignition is expected. However, no PLIF signal is detected near the injector region which would indicate first-stage ignition products due to the higher ambient temperature. The simulation, on the other hand, clearly predicts a high amount of first-stage ignition products in the form of formaldehyde. Moreover, due to the existence of high temperature products of the first injection, second-stage ignition of the second spray head is accelerated and also
5.5. Case 1 (900 K): Reactive Simulation and Comparison to the Experiment

Acetylene is formed. The fast transition could be caused due to the chemical reaction mechanism or the reinitialization model.

In the box of 1.2 ms ASOI, a PLIF signal is observed between an axial distance of 13 and 28 mm. The lift-off length associated with the second injection (also seen in figure 5.20) is approximately 13 mm and therefore closer to the injector than the one from the first injection. It has been assumed that the PLIF signal observed between 13 and 15 mm is caused by formaldehyde, whereas the signal beyond 20 mm might be due to early formation of PAH [55]. Considering the simulation, the second spray head has a penetration length of 22 mm. In the whole rich core of the spray, high amounts of formaldehyde are predicted. After 11 mm, the amount of C$_2$H$_2$ rises significantly (seen by the red colour) and indicates therefore a lift-off of about 11 mm.

![Figure 5.21: Time sequence of 355 nm PLIF compared with the computed contour plots of formaldehyde and acetylene (taken as a qualitative replacement for PAH), single realization. Order of the plots: first plot shows experimental results (µs in title) with direct comparison to the simulation (ms in title) arranged below. The white solid and dotted lines show iso-contours of stoichiometric (\(\xi_{st} = 0.0463\)) mixture fraction and the spray border (\(\xi = 0.01\)), respectively. Experimental data from [55]. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_2$.](image)
The hypothesis with the detection of the soot precursor is supported by the PLIF image at 1.5 ms ASOI. The signal intensity after 20 mm increases compared to the more upstream signal and is therefore believed to originate from PAH. In contrast to the PLIF image at 0.7 ms ASOI, a broader area of PAH signal is detected, which indicates an increased rate of PAH formation for the second injection. This is most likely due to the earlier second-stage ignition of the second injection, occurring in a more fuel-rich region than for the first injection. However, the radial width is again underestimated. The simulation now predicts a correct lift-off length, if the beginning of the red coloured area of the soot precursor is taken as a qualitative indicator. Like it was seen during the first injection, formaldehyde is not completely consumed and is present also after the lift-off length, having a decreasing tendency towards farther axial distances. Comparing the amount of soot precursor to the first injection (at 0.7 ms), a considerably higher amount is predicted, which is in accordance to the experiment.

The last PLIF image at 1.7 ms ASOI shows mainly high temperature combustion with a very high signal of PAH. The spatial distribution is extended from about 25 to 48 mm, showing constant high intensity. The simulation predicts a thinner soot cloud, which we believe is due to the computation of the flow field. A high amount of soot precursor is observed up to 48 mm, which is in reasonable accordance to the PLIF image. However, the soot precursor is also present upstream of 25 mm.

### 5.5.5 Total Soot Mass

The computation of soot is not the general focus of this project, however it is included in the simulation. Soot modelling is presented in detail in [4, 6] and is not repeated here for brevity. The ensemble average of total soot mass of four realizations is shown in figure 5.22. The solid black line with the dots shows the ensemble average of the experiment and the red solid line illustrates the ensemble average of the LES-CMC simulation, whereas the yellow and pink shaded areas indicate the shot-to-shot variations. Based on the experimental data [53], it is known that the second injection produces a factor of four times more soot than the first injection. This effect is mainly caused by the early ignition of the second injection, which occurs near the liquid fuel core under more fuel-rich conditions. As shown in figure 5.22, the soot-mass-prediction of the LES-CMC simulation is slightly out of bounds and too low for the first injection, whereas the simulation remains more consistent to the experiment at later timings. The simulated maximum averaged total soot mass 2.0 ms ASOI was around 9 µg, whereas the experimental one was found as 7.5 µg.

![Figure 5.22: Experimental and simulated total soot mass for split injection schedule (0.5/0.5 dwell/0.5 ms) at the Spray A ambient conditions. Experimental data from [53].](image)
5.6 Reactive Simulation by Direct Integration Combustion Model

As a comparative measure, the split injection was also simulated by means of the direct integration combustion model. The same ambient gas conditions and initial conditions have been chosen like in the LES-CMC setup. Since DI considers the control volumes as well-mixed, reactions are limited to areas close to stoichiometry. Since there is no scalar dissipation rate which describes molecular mixing, oxygen is unlikely to diffuse inside the spray core and is rather consumed at the flame front [4]. In contrast, the combustion model CMC always computes PDF-distributions for the species, which increases the probability of oxygen in the fuel-rich part of the spray. These effects are illustrated in figure 5.23 and therefore, a different combustion behaviour is expected.

![Oxygen mass fraction computed with CMC.](image1)

![Oxygen mass fraction computed with Direct Integration.](image2)

Figure 5.23: Contour plots of oxygen mass fraction computed 0.6 ms ASOI. The left plot shows higher amount of oxygen in the fuel-rich part of the spray (i.e. spray core) than the right one.

5.6.1 Pressure Rise

First of all, the pressure rise is taken as qualitative indicator for combustion. In figure 5.24, the comparison of the pressure rise between the experiment, the LES-CMC and LES-DI simulation is illustrated. The pressure rise of LES-DI fits better to the experiment than LES-CMC. The pressure starts to rise around 0.2 ms ASOI, and shows approximately an equal rate of pressure rise as LES-CMC. After 1.0 ms ASOI, the total pressure rise of the experiment is about 11 kPa, about 9 kPa for LES-DI, and 8 kPa for LES-CMC. For the second injection, the rate of pressure rise for LES-DI is higher than for LES-CMC. After 2.0 ms ASOI, the total pressure rise of the experiment is about 25 kPa, 21.5 kPa for LES-DI and around 16 kPa for LES-CMC. It has to be noted that both simulation types fail to achieve the correct total amount of pressure rise, whereas the prediction of LES-DI is more consistent than the one of LES-CMC. A possible reason for the lack of correct prediction of the pressure rise could be a different total volume (caused by the injector, intake/exhaust valve, etc.), comparing the combustion vessel with the computational domain of the simulation. From the above-mentioned findings, it can be concluded that the direct integration model leads to a faster, stronger combustion than with LES-CMC. This hypothesis is supported by the comparison of the contour plots of OH of both LES-CMC (figure A.3, appendix) and LES-DI (figure A.5 appendix): Figure A.5 shows higher penetration lengths than figure A.3, however, the radial width appears to be similar. This means that the DI-simulation is mixing faster and that the available volume of the spray which can react is higher compared to CMC, or that the expansion of the flame in axial direction is faster than the one from CMC. This effect is observed in the mentioned figures, since the (non-reactive) penetration lengths of the two sprays seem to be identical up to ignition. After ignition, the spray computed by DI seems to penetrate faster into the combustion chamber than the one computed by CMC, and therefore, the amount of reacting control volumes is bigger compared to CMC. Hence, the pressure rise of DI is higher.
Chapter 5. Results and Discussion

5.6.2 Comparison of C₂H₂ and CH₂O to 355 nm PLIF

Like it was seen before, figure 5.25 shows a time sequence of PLIF images compared to contour plots of C₂H₂ (soot precursor, upper half) and CH₂O (lower half). The detailed description of the experiment can be read in section 5.5.4 and is not repeated here, only the findings from the simulation are commented. Note that the signal intensity from the experiment and the colour scales of CH₂O and C₂H₂ are not necessarily the same, and the latter two differ by a factor of four.

Starting at 0.7 ms ASOI, it is visible that nearly all formaldehyde has already been consumed, whereas in the experiment formaldehyde is observed at the lift-off length of 16 mm. Additionally, high amounts of soot precursor are predicted at further axial distances than 12 mm, while the experiment only shows a high intensity signal at the spray tip.

1.0 ms ASOI, most parts of the soot is already oxidized and only a small zone of C₂H₂ remains. The experiment however still shows a strong signal from PAH.

The contour plot at 1.1 ms ASOI or 0.1 ms after the start of the second injection, the CH₂O of the second spray penetrated approximately 19 mm, which is too far compared to the experiment. The second injection penetrates into high temperature combustion products of the first injection, therefore the transition into second-stage ignition is accelerated, leading to the prediction of soot precursor near the injector. However, the amount of C₂H₂ at this time is not as high as it was seen with LES-CMC. The simulation predicts advanced cool-flame reactions, indicated by formaldehyde close to the nozzle, whereas the experiment shows no PLIF signal in that zone at this time.

The PLIF signal at 1.2 ms ASOI contains both formaldehyde (at 13-15 mm axial distance) and PAH (beyond 20 mm axial distance) and a shorter lift-off length at 13 mm as the first injection. In the simulation, formaldehyde is present on the whole length of the spray, i.e. it is not consumed at the lift-off length. The soot precursor is mainly present after 10 mm, but indicates no flame lift-off like it was the case with LES-CMC.

The PLIF image at 1.5 ms ASOI shows a formaldehyde signal after 13 mm and a PAH signal
after 20 mm until 35 mm (distinguished by the signal intensity). The simulation shows that the penetration length of the second injection is too long, it is 50 mm, whereas it should be around 35 mm. A considerable amount of formaldehyde is predicted up to an axial distance of 30 mm, and at farther distances, the amount of soot precursor is high. The general observation of having CH$_2$O at the flame base and C$_2$H$_2$ in the spray tip is reasonable, however, the corresponding location is questionable.

In the last PLIF box at 1.7 ms, the signal from PAH is very intense (i.e. higher than at 0.7 ms for the first injection), is extended from 25 to 48 mm and is caused by the earlier ignition of the second injection. In the simulation, formaldehyde has mostly been consumed and only a thin, narrow soot precursor cloud prevails. However, it is difficult to evaluate, if the amount of C$_2$H$_2$ for the second injection is considerably higher than for the first injection. Furthermore, the reactive penetration length is over-predicted by approximately 20 % and is too narrow.

Figure 5.25: Time sequence of 355 nm PLIF compared with the computed contour plots of formaldehyde and acetylene (taken as a qualitative replacement for PAH) using direct integration, single realization. Order of the plots: first plot shows experimental results (µs in title) with direct comparison to the simulation (ms in title) arranged below. Experimental data from [55]. Ambient conditions: 900 K, 22.8 kg/m$^3$, 15 % O$_2$. 
5.6.3 Comparison of Density Plots to Schlieren Images, Reactive Setup

The comparison of contour plots of density with schlieren images is shown in figure 5.26. The arrangement of the plots is as it was seen before. The reactive penetration length of the first injection seems to be captured well up to 1.2 ms, afterwards it is over-predicted to a small extent. The reactive penetration length of the second injection, on the other hand, is mostly overestimated.

Starting at 1.2 ms, the prediction seems to be accurate. Afterwards, the second injection penetrates too fast into the computational domain. As it was mentioned before, the reaction zone of the second injection (indicated by the formaldehyde and acetylene iso-contours) is generally too narrow. It appears that the prediction deteriorates with time, observing a difference of approximately 10 mm
5.6. Reactive Simulation by Direct Integration Combustion Model

Comparing the experimental and the simulated penetration length of the second injection at 1.7 ms. To conclude, the direct integration combustion model predicts a correct reactive first penetration length, but shows immense weaknesses in computing the second reactive injection.

5.6.4 Computational Cost

The computational costs of using either a structured 2D-CMC grid or direct integration are very different and shown in detail in Table 5.3. Since the fine CMC discretization type always considers 8 CFD cells per one CMC cell, and the azimuthal direction is collapsed onto one single plane, the computation is much cheaper. The direct integration considers the chemical reactions in each CFD cell separately, and is therefore very expensive. Despite the fact that CMC uses a coarser resolution for the computation of chemical reactions than direct integration, the CFD cells are treated individually in the sense that they all contain a different β-PDF distribution and therefore, different species mass fractions and temperatures. An additional advantage of CMC is that turbulence-chemistry interactions are taken into account, whereas they are neglected in direct integration.

Table 5.3 clearly shows that the simulation using DI was around 6 times more expensive than the one using CMC. Therefore it can be concluded, that not only the computational cost is tremendously reduced by using the CMC model, but also the results appear to be more accurate for the split injection setup. Finally, a CFD mesh refinement is most likely necessary and could improve the quality of the results.

<table>
<thead>
<tr>
<th></th>
<th>2D-CMCfine</th>
<th>Direct Integration</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of nodes/cells</td>
<td>2'424</td>
<td>~1'900'000</td>
</tr>
<tr>
<td>2 ms total CPU time [h]</td>
<td>114.6</td>
<td>271</td>
</tr>
<tr>
<td>Number of processors</td>
<td>96</td>
<td>248</td>
</tr>
<tr>
<td>Total hours/proc. [h]</td>
<td>11'000</td>
<td>67'200</td>
</tr>
<tr>
<td>Ratio</td>
<td>100 %</td>
<td>611 %</td>
</tr>
</tbody>
</table>

5.6.5 Additional Considerations

A closer look to the appendix, where the detailed time evolution of temperature and OH is illustrated (figures A.4 and A.5), leads to the conclusion that second-stage ignition occurred at the sides of the spray. Since the identical effect was observed in LES-CMC, it could be possible that a CFD-mesh-convergence has not been reached yet. A refined CFD-mesh might lead to the wanted effect of main ignition at the spray tip. The most obvious difference, after comparison with LES-CMC (figure A.2), is that the combustion is more advanced, i.e. more high temperature zones (indicated by the red colour) are observed. Moreover, the mass fractions of OH are much more concentrated to stoichiometric mixtures than with LES-CMC (fig. A.3). This is caused by the direct integration combustion model, like it was mentioned before.
Chapter 5. Results and Discussion

5.7 Case 2 (750 K): Reactive Simulation and Comparison to Experiment

The flow field of the spray was tuned earlier for Case 1 and the CMC grid sensitivity analysis showed that the fine resolution exhibits the best advantage-to-cost ratio. An additional flow field validation for Case 2 was not necessary, since the ambient density is identical to the one of Case 1 and therefore, the non-reactive vapour penetration length is expected to be the same. Furthermore, the identical CMC grid was applied (2D-CMCfine).

5.7.1 Ignition Delay

The ignition delay was again computed according to the equation 5.1. The maximum temperature is therefore illustrated in figure 5.27. During the experiment [55], an ignition delay of \( \tau_{\text{ID,exp}} = 2.0 \pm 0.05 \text{ ms} \) was measured, whereas the simulation showed an ignition delay of \( \tau_{\text{ID,sim}} = 1.83 \text{ ms} \), which is within a \( \pm 9 \% \) range compared to the experiment. Moreover, in [55] it is stated that the ignition timing showed a large variability at the 750 K ambient condition. From the plot below it is clearly visible that shortly before 1.5 ms ASOI, the mixture undergoes first-stage ignition, which causes a temperature rise to 850-900 K. Shortly later, second-stage ignition is initiated and the maximum temperature rises towards 2120 K, therefore the jump in maximum temperature is approximately 1370 K. This is around 50 K higher compared to case one and is most likely caused by the higher pressure gradient for the LTC-case.

![Figure 5.27: Time evolution of the maximum temperature of Case 2. The dashed line is the split injection profile.](image_url)

5.7.2 Evolution of Temperature Conditional on Mixture Fraction

In figure 5.28, the temperature conditional on mixture fraction is plotted for Case 1 and Case 2. The differences are obvious: 1) Like it was reported before, first-stage ignition (around 0.2 ms) occurs in fuel-rich zones for Case 1, whereas for Case 2, it happens around lean to stoichiometric mixtures. 2) Second-stage ignition (between 0.3 ms and 0.4 ms) happens in fuel-rich zones (around \( \xi = 0.09 \)) for Case 1, propagating towards stoichiometry at later stages. For Case 2, second-stage ignition happens around stoichiometry and only slightly rich parts (seen at 1.8 ms), the peak value at later stages is also seen at stoichiometric values. 3) For Case 1, the main ignition event happens
5.7. Case 2 (750 K): Reactive Simulation and Comparison to Experiment

during the first injection shortly before 0.4 ms, whereas it happens after the end of the second injection for Case 2, shortly before 1.9 ms. 4) Considering 1.0 ms (0.65 ms after ignition) of Case 1, the burning process is still going on, because there are still rich parts of fuel, which are going to be consumed by the flame. For the LTC-like condition, the plot at 2.3 ms (0.45 ms after ignition) shows almost no rich hot zones anymore and therefore, the combustion process is almost over. In the last plot of the simulation (2.475 ms), some single fuel-rich cells are observed at medium temperature (around 1300 K), which are most likely not undergoing second-stage ignition and lead to a low combustion efficiency.

5.7.3 Pressure Rise

The black solid line with dots in figure 5.29 shows the normalized total pressure rise from the experiment [55] (realization "D" of Skeen et al. was considered) and the red solid line illustrates the pressure rise from the LES-CMC computation. Since the total pressure rise was not available, the normalized pressure is plotted, where the maximum pressure rise up to almost 2.5 ms ASOI was considered as the scaling variable. It has to be noted that in the simulation the evaporation of the spray lowers the internal chamber pressure more than the experiment. Moreover, the experimental pressure starts to rise considerably after 1.4 ms ASOI, whereas the computed pressure increases mainly after 1.8 ms. The simulated pressure evolution shows generally a reasonable trend compared to the experiment.

Figure 5.28: Evolution in time of temperature conditional on mixture fraction for the whole computational domain, comparison between Case 1 and Case 2. The dashed-dotted lines indicate $\xi_{st}$.
Figure 5.29: Pressure rise evolution of Case 2, comparison between the normalized pressure of the simulation and the experiment. Black solid line with dots: experiment, red solid line: LES-CMC simulation, black dashed line: split injection profile. Ambient conditions: 750 K, 22.8 kg/m³, 15 % O₂. Experimental data from [55], realization "D".

5.7.4 Apparent Heat Release Rate

The normalized AHRR is plotted in figure 5.30. The black line with dots shows the experimental data (realization "D" of [55] was considered) and the blue line shows the simulation by LES-CMC. The experimental heat release commences at 1.2 ms ASOI, most likely due to the initiation of cool-flame reactions. This first bump in the heat release is caused by the ignition of a premixed fuel-air mixture, which was formed during the non-igniting first injection and the beginning of the second injection. This first-stage ignition is clearly related to a chemical ignition delay. The main heat release follows shortly later and has its peak at 2.0 ms ASOI and is related to second-stage ignition. The simulation on the other hand exhibits a much smaller portion of heat release belonging to first-stage ignition. Like it was already seen in Case 1 (figure 5.19), the heat release from the first-stage ignition is rather small. This might be caused by the chemical mechanism since it is known, that
low temperature reactions are difficult to capture accurately. It has to be noted that the maximal heat release rate in the experiment was measured as approximately 108 J/ms, whereas the one from the simulation was computed as 61 J/ms (not shown here). The issue is most likely the problematic prediction of the pressure rise, which is clearly correlated with the heat release rate. A further cause might be the chemical mechanism, since it calculates the specific heat capacity $c_p$. Further effort has to be dedicated to this topic.

### 5.7.5 Comparison of Density plots to Schlieren images

A single realization of Case 2 in comparison with schlieren images is shown in figure 5.31. The comparison always begins with an experimental image with the corresponding contour plot below and the specific timings are indicated in the upper left corner. In the schlieren images, the red line indicates the boundary from the PLIF signal and shows the location of formaldehyde occurrence. The red lines in the simulation contour plots indicate iso-contours of formaldehyde and acetylene, the black dotted lines show iso-contours of the leanest mixture fraction to indicate the spray border and the white solid lines illustrate iso-contour of stoichiometric mixture fraction to indicate the position of the second injection. It has to be noted that the simulation was restarted after the time step 2.48 ms, which led to a questionable computation of pressure and density. Hence, the comparison at 2.7 ms was left out.

![Figure 5.31: Time sequence of schlieren images compared with the computed contour plots of density, single realization. Order of the plots: first plot shows experimental results ($\mu$s in title) with direct comparison to the simulation (ms in title) arranged below. In the experimental images, the red lines indicate the location from the 355-nm CH$_2$O PLIF signal. In the simulation plots, the red solid, black dotted and white solid lines show iso-contours of formaldehyde plus acetylene ($Y_{CH_2O} + YC_2H_2 = 0.001$), the mixture fraction of the spray border ($\xi = 0.01$) and the stoichiometry, respectively. Experimental data from [55]. 750 K ambient condition.](image)

The first schlieren plot at 1.5 ms ASOI shows that the fuel from the first spray has mostly evaporated which is indicated by a mixture that is nearly transparent to the schlieren effect. According to [55], this is also not an indicator of first-stage ignition for the 750 K ambient case. The simulation shows a very good agreement to the experiment, since the penetration length of both the
first and the second injection within a ±2 mm range. A formaldehyde iso-contour (acetylene is not present anyway) is also not visible at this point in time, which is associated with a low-reacting state.

The box at 1.7 ms ASOI shows a mild darkening of the schlieren effect, which indicates first-stage ignition. The simulation shows also a decreasing density which is correlated to cool-flame reactions. However, the darkening in the contour plot covers a smaller area than in the experiment. The penetration lengths seem to be very accurate at this time step, however, the radial spreading is under-predicted, which causes the low density zone to appear smaller than in the experiment.

The next pair of images at 1.8 ms exhibits a further darkening of the schlieren effect and the density contour plot, respectively. It is observed that the reaction zone in the simulation is more concentrated to the centre axis. In contrast to the 900 K ambient case, it was found that the second injection of the experiment was observed more concentrated to the spray axis. This suggests that the second spray, entering the slipstream effect of the first injection, is exposed to faster penetration, less radial mixing and a smaller spreading angle [55]. This effect is likely to be over-predicted by the simulation.

The last two boxes at 2.1 ms show that high temperature ignition occurred, which is illustrated by the dark colour in both the experiment and the simulation. The penetration length of the first injection seems to be slightly too short assuming that the smaller reaction zone leads to less thermal expansion. The penetration length of the second spray is still predicted accurately. The computation of the penetration lengths looks generally reasonable. Further investigation concerning the ignition behaviour is described below in the section where the PLIF images are analysed.

5.7.6 Comparison of CH2O to 355 nm PLIF

In order to analyse the combustion process elaborately, a time sequence of PLIF images is again compared to simulation contour plots of formaldehyde in figure 5.32. Note that this PLIF signal does not suffer from interference due to PAH, since the 750 K ambient case appears free of soot formation [55]. The PLIF images were taken from five unique experiments with identical ambient conditions (indicated by the capital letters in the upper right corner), which showed large variability in ignition timing. The order and the description of the plots follows the one from figure 5.21. Beginning at 1.5 ms ASOI, the experiment shows no PLIF signal, which indicates no cool-flame reactions. The formaldehyde contour plot shows slight blue areas. However, the amount of formaldehyde is negligibly small for this time step, which indicates that no advanced cool-flame reactions have occurred.

The next PLIF frame (1.7 ms ASOI) shows a slightly intensified formaldehyde signal which indicates first-stage ignition. Together with the second set of boxes in figure 5.31 where the schlieren effect from the first injection mildly darkens, the hypothesis is supported that the second injection mixes with cool-flame products prior to its ignition [55]. This effect is also seen in the simulation, where first-stage ignition occurs downstream of 40 mm and the second spray head starts to mix with the cool-flame products.

Later at 1.8 ms ASOI, the PLIF signal shows an increased intensity which indicates that first-stage ignition has occurred for the second injection [55]. It has to be noted that the reactive intermediates produced during the first injection enhance the reactivity of the second injection. The simulation also shows higher amount of formaldehyde at this timing, the reaction zone is, however, considerably smaller. A further observation is that the reaction zone at the tail of the first experimental spray (about 25 to 35 mm) is divided by the incoming second injection. This effect is predicted well by LES-CMC.

In the fourth set of boxes at 2.1 ms ASOI, second-stage ignition occurred and formaldehyde is continuously consumed which is indicated by the gap after 45 mm, which is downstream of the penetration distance of the second injection. It is therefore not possible to determine whether high temperature ignition occurs first for the second or the first fuel spray, but it clearly indicates that the earliest second-stage ignition event is enabled by the second injection. This finding is well replicated by the simulation, which ignites slightly too far upstream, but clearly due to the second injection, which might be the most important feature to be predicted. The contour plots illustrate
that wherever there is stoichiometric to fuel-rich mixture, formaldehyde is consumed and high temperature combustion is observed (also seen in the appendix, by the temperature in figure A.6 b) and by OH in figure A.7 b)).

The last PLIF image at 2.7 ms ASOI shows advanced high temperature combustion, however the far upstream zone around 30 mm shows large quantities of formaldehyde. These zones indicate broad and persistent zones of incomplete combustion. The schlieren image, which is not shown here, lacks of a darkening schlieren effect at the tail of the spray which correlates to low temperature of the combustion products and a lack of combustion recession. The 750 K ambient case generally showed poor combustion efficiency [55]. The simulation also shows incomplete combustion at the tail of the spray and at lateral region at 50 mm axial distance, which is in similar to the experiment. The qualitative outcome of this investigation is predominantly satisfactory and is very promising in terms of simulating LTC/PCCI in the feature.

![Figure 5.32: Time sequence of 355 nm PLIF compared with the computed contour plots of formaldehyde, single realization. Order of the plots: first plot shows experimental results (µs in title) with direct comparison to the simulation (ms in title) arranged below. The white solid and dotted lines show iso-contours of stoichiometric ($\xi_{st}=0.0463$) mixture fraction and the spray border ($\xi=0.01$), respectively. Experimental data from [55]. 750 K ambient condition.](image)

5.7.7 Total Soot Mass

Like it was mentioned before, the 750 K ambient temperature experiment appeared free of soot. The same effect was seen in the simulation, where the total soot mass peaked around a value of 0.006 µg at 2.3 ms ASOI, which is more than three orders of magnitude lower than in the 900 K ambient case. During the whole simulation, the amount of computed soot precursor ($C_2H_2$) was almost negligible as it is illustrated in the appendix (figure A.7 a)). The low formation of the pollutant soot is an intentional effect, which is caused by the strong mixing of fuel and air before ignition, leading to very fuel-lean conditions at the time of high temperature combustion.
Chapter 6
Conclusions and Outlook

A reacting spray flame, namely the Spray A split injection setup of the ECN using \( n \)-dodecane fuel, was modelled employing the state-of-the-art CMC model on a structured grid with detailed chemistry in conjunction with an LES model using a three-dimensional mesh. Both meshes are highly resolved in areas of the nozzle and around the spray. A non-reactive spray calibration was carried out for the first and second injection in order to achieve correct prediction of the vapour penetration length. Additionally, the reactive penetration length of the first injection was evaluated. Three different CMC grid resolutions, i.e. a one-dimensional, a coarse and a fine two-dimensional grid, were examined by comparison of ignition delay, ignition location, flame structure development, temperature conditional on mixture fraction and computational cost. Additionally, the ignition process is studied in detail for the LES-CMC approach. Here, the best CMC grid was determined for the following simulations. The CMC reinitialization model was analysed in detail as well as the ignition behaviour of the second injection. An ensemble average consisting of five realizations was achieved for the complete Spray A split injection having 900 K ambient condition (Case 1, diesel-like condition). Direct comparison of the numerical results to the experimental data was accomplished in terms of pressure rise, AHRR, schlieren images, 355 nm PLIF and the total soot mass. As a complementary measure, the split injection setup was modelled applying the direct integration combustion model using the identical CFD-mesh and skeletal reaction mechanism. The two modelling approaches LES-CMC and LES-DI were compared to each other. Finally the LES-CMC setup was used to model the 750 K ambient condition (Case 2, LTC-like condition). One realization was accomplished in order to compare the simulation with the different measurements. The findings, which were deduced from the LES-CMC as well as the LES-DI model, are described in the following.

6.1 Spray Calibration and CMC grid sensitivity Analysis

The comparison of the experimental and simulated non-reactive vapour penetration length showed that both injection lengths are correctly predicted and hence, also the slipstream effect of the first injection. The assessment of the reactive penetration length was in good accordance to the experiment. The ignition delays were computed and compared to the experimental value of 0.35 ± 0.01 ms and resulted in +12 %, +2.6 % and +0.6 % deviation for the 1D-CMC, 2D-CMC coarse and 2D-CMC fine case, respectively. The distribution of formaldehyde and temperature during the ignition process was physically the most realistic for the fine 2D-CMC grid. A further observation during transition from low to high temperature combustion around 0.7 ms ASOI was that the soot precursor \( \text{C}_2\text{H}_2 \) was seen evenly distributed for the latter grid, whereas the other two grids showed questionable patterns. The examination of the conditional mean temperature around 0.7 ms ASOI demonstrated a physically wrong cut-off for the one-dimensional grid (i.e. the temperature is jumping from low to high temperature comparing one to the other axial location), the two-dimensional grids exhibited, on the other hand, a transition including large scale fluctuations, which corresponds well to the literature. Further evaluations of contour plots at 1.0 ms ASOI
showed that the highest magnitude of soot mass fraction and the most realistic shape and location of the soot cloud was predicted by the fine, two-dimensional CMC grid. An additional aspect to consider was the thermal expansion. It was found to take place mostly in axial direction, the radial expansion was underestimated by all discretization types, none of them showing a clear advantage. Detailed investigation of the temperature conditional on mixture fraction led to the conclusion that ignition is initiated in lean mixtures, propagates into rich mixture zones to undergo low temperature combustion and travels back towards stoichiometric fuel/air mixtures, where high temperature combustion occurs. However, the fastest transition from low to high temperature combustion was seen by the fine 2D-CMC type. Furthermore, the quantitative pressure rise showed no evidence for choosing the fine over the coarse CMC grid resolution. The computational expenses increased roughly 60% between the 1D and coarse 2D mesh refinements, and around 100% between the 1D and the fine 2D grid. In conclusion, the use of the fine 2D-CMC grid results in a highly detailed structure of a lifted flame and has therefore the best advantage-to-cost ratio.

6.2 Case 1 (900 K): Reactive Simulation using LES-CMC and Comparison to the Experiment

Unless stated otherwise, LES-CMC simulations are considered. The quantitative evaluation of the internal chamber pressure showed that the numerical result is 34% below the measurement. However, the qualitative pressure rise seems to be accurate, it remains to check if the reason for the weak quantitative prediction comes from the CMC combustion model, the turbulence model (mixing issue), uncertainty of the volume or the injected fuel mass. Since the AHRR is closely connected to the pressure, its evolution shows similar trends and is slightly below the experimental one, the trend is correct however. The AHRR-based ignition delay of the second injection was computed as $0.15 \pm 0.07$ ms, whereas it is $0.17 \pm 0.01$ ms in the experiment. Therefore, the ignition delay of both the first and the second injection was computed very accurately. The qualitative comparison of density contour plots to schlieren images resulted in accurate predictions of the penetration lengths with only slight deviation from the simulated second injection. The general outcome is satisfactory, however, weaknesses were observed in terms of radial spreading, which could be enhanced by additional CFD-mesh refinement as it was seen by Pei et al. [45].

A next measure was to compare PLIF images with contour plots of formaldehyde ($\text{CH}_2\text{O}$) and acetylene (soot precursor, $\text{C}_2\text{H}_2$). Difficulty in capturing the lift-off length at early points in time as well as an early appearance of soot precursor during the second injection was observed. However, the overall qualitative prediction of formaldehyde and soot precursor was accurate and a main feature of the second injection, having more soot than the first one due to its earlier ignition, was captured. Temperature and OH plots showed that main ignition occurs mainly at the sides of the spray, whereas in the experiment it happens in a large volumetric area at the spray tip. The soot-mass-prediction of the LES-CMC simulation is too low for the first injection and slightly too high for the second injection ($9 \, \mu\text{g}$ versus $7.5 \, \mu\text{g}$ at 2.0 ms ASOI). The time evolution of soot is generally too early, but shows good agreement.

6.3 Case 1 (900 K): Reactive Simulation using LES-DI and Comparison to the Experiment

The pressure rise computed by LES-DI demonstrated better agreement to the experimental data. The total pressure rise was 25 kPa for the experiment, 21.5 kPa for LES-DI and 16 kPa for LES-CMC. Therefore, the hypothesis is supported that the DI-model leads to faster, stronger combustion than the CMC-model due to its nature of a $\delta$-function, and often this means that DI tends to overestimate combustion events in comparison to CMC. Further analysis of combustion quality in terms of formaldehyde and soot precursor prediction showed that the lift-off length of the experiment could not be predicted. Schlieren images compared to density plots indicated that the penetration length is also overestimated due to its intensified combustion. Furthermore, the
predictions of C\textsubscript{2}H\textsubscript{2} indicated questionable locations and shapes of the soot cloud. In addition, contour plots of temperature and OH showed that the main high temperature ignition occurs at the sides of the spray, similarly to the CMC model. This finding indicates that the ignition location is most likely an issue of the CFD-mesh and that convergence has not been reached yet. To conclude, the direct integration combustion model predicts a higher intensity of combustion and therefore pressure rise, the flame structure and development was however seen qualitatively better while using LES-CMC. After all, the computational costs of same setup using DI instead of CMC are around six times higher.

6.4 Case 2 (750 K): Reactive Simulation using LES-CMC and Comparison to the Experiment

Due to the lack of the quantitative pressure rise for Case 2 and due to the fact that only one realization of the simulation was available, the comparison was done qualitatively. Hence, the normalized pressure was compared. The experimental pressure starts to rise earlier than the simulation suggesting that the low temperature reactions of the chemical mechanism lead to poor heat release. The shape and the time evolution of the AHRR was mainly consistent, however the amplitude is considerably below the measurement (108 versus 61 J/ms peak AHRR for the experiment and the simulation, respectively). Presumably, this is the same issue like it was seen in Case 1. The comparison of the simulation to schlieren plots showed generally accurate predictions of the penetration lengths. Again, the computed thermal expansion is too weak. The experimental ignition delay was measured as \(2.0 \pm 0.05\) ms, whereas it was computed as 1.83 ms, which is within a \(\pm 9\%\) range compared to the experiment. However, since Skeen et al. [55] reported large shot-to-shot variability in ignition timing at the 750 K ambient condition, the computed ignition delay is within the margin of error. The detailed ignition behaviour was analysed by comparison with PLIF images. The simulation indicates that the second injection mixes with cool-flame products of the first injection which leads to increased reactivity. Furthermore, it was observed that the earliest second-stage ignition event is enabled by the second injection, which was seen accordingly in the experiment. No combustion recession was observed neither in the experiment nor in the simulation under this condition. Generally, this split-injection scenario demonstrates poor combustion efficiency, i.e. in the experiment only 75 \% of the fuel energy was released and the computed cumulative AHRR is estimated even below. Nevertheless, it appears unlikely that a single 0.5-ms injection would ignite in an engine relevant time scale [55]. Under the 750 K ambient condition, this would lead to even more unburned hydrocarbons and a very low combustion efficiency. The split injection setup opens new possibilities in low load operating conditions of an engine such as cold-start or engine idle conditions. The 750 K ambient condition case appeared free of soot both in the experiment and the simulation which is caused by the very fuel-lean conditions during high temperature combustion. The computational expenses increased by 6 \% compared to Case 1, having 2.7 ms total simulation time instead of only 2.0 ms, because second-stage ignition happens later.

6.5 Closing Words and Outlook

The report enables to gain further knowledge concerning detailed modelling of the Spray A split injection using LES-CMC. The findings of this project are very encouraging for future research and provide a solid basis in terms of the numerical simulation of auto-igniting diesel sprays at engine-relevant operating conditions, employing modern combustion strategies such as LTC. This work delivers detailed understanding of the combustion process of a highly transient multiple injection setup. The numerical setup used for investigation of spray combustion under conventional diesel-like conditions was used for studying a split injection schedule at LTC-like conditions with reduced bulk temperature at start of injection. This is a very promising approach to direct the engine development towards new, cleaner techniques. The possibility of a diesel engine under
LTC-like conditions is a further step towards premixed charge compression ignition (PCCI), where several pilot injections ensure ignition of the main injection under otherwise unfavourable ambient conditions, such as low bulk temperature, which results in lowering engine-out emissions. Further investigations concerning the development of models for PCCI-combustion are strongly recommended.
Appendix A

Contour Plots of simulated Split Injection by LES-CMC and DI

The first three plots show an ensemble average of the LES-CMC simulation. The detailed time evolution of mixture fraction, temperature and the radical OH for Case 1 is illustrated in figures A.1-A.3. Furthermore, one realization of direct integration has been carried out for Case 1. The time evolution of temperature and the radical OH is visible in figures A.4 and A.5. Finally the contour plots of Case 2 are shown, the time evolution of mixture fraction, temperature, soot precursor (C$_2$H$_2$) and the radical OH are illustrated in figures A.6 and A.7.
Figure A.1: LES/2D-CMCfine NX=12 NY=1 NZ=202: Mixture Fraction Ensemble Average (n=5), split injection setup. The white line illustrates the stoichiometric mixture fraction. 900 K ambient condition.
Appendix A. Contour Plots of simulated Split Injection by LES-CMC and DI

Figure A.2: LES/2D-CMCfine NX=12 NY=1 NZ=202: Temperature Ensemble Average (n=5), split injection setup. The white line illustrates the stoichiometric mixture fraction. 900 K ambient condition.
Figure A.3: LES/2D-CMC fine NX=12 NY=1 NZ=202: OH Ensemble Average (n=5), split injection setup. The white line illustrates the stoichiometric mixture fraction. 900 K ambient condition.
Figure A.4: LES-direct-integration, contour plots of temperature, split injection setup. 900 K ambient condition.
Figure A.5: LES-direct-integration, contour plots of OH, split injection setup. 900 K ambient condition.
Figure A.6: Time evolution of mixture fraction and temperature. 750 K ambient condition.
Figure A.7: Time evolution of acetylene and OH mass fractions. 750 K ambient condition. From the OH plot it is seen that OH-reactions occur only at stoichiometric to lean conditions, since the spray has such a long time to lean out. This is a very different behaviour compared to the 900 K ambient condition, where OH is also formed at fuel-rich regions.
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