High-performance Gasoline Direct Injection engine - 3D-CFD spray and combustion simulation

Supervisors:
Prof. Federico MILLO
Prof. Luciano ROLANDO
PhD Andrea PIANO

Candidate:
Andrea SCALAMBRO

December 2020
Abstract

Nowadays the development of new internal combustion engines is significantly growing in complexity because of the challenging targets set by the governments and by the customer on its pollutant emissions and performance respectively. Moreover, the huge number of competitors in the automotive sector forces car manufacturers to strongly reduce the lead time of their new product in order to maintain a satisfactory level of profitability. Therefore, the development of reliable and predictive simulation tools is becoming crucial to investigate a wide range of innovative technical solutions and to reduce the number of expensive experimental campaign.

In such a framework the goal of this thesis is the development of a 3D CFD model capable to reproduce the in-cylinder phenomena of a high-performance Direct Injection Spark Ignition Engine. The work, performed on the software Converge CFD (V2.4), is mainly divided into two parts. The first one focuses on the calibration of the injection spray model. Experimental measurements and optical characterization of the injector over different operating conditions were used to properly tune the calibration parameters of the subroutines for Primary and secondary breakups, transport and evaporation phenomena. The Reynolds Averaged Navier-Stokes (RANS) along with the RNG $k-\varepsilon$ turbulence model was employed to account for fluctuations of field variables. In this phase the definition of main grid settings was also performed.

The second part deals with the simulation of the entire engine cycle and in particular of the combustion process. The firing cycle simulation was preceded by the cold cycle simulation to validate the gas exchange processes, wall heat transfer and orientation and distribution of the injected spray inside the combustion chamber. Regarding the firing cycle, a detailed chemical kinetics solver (SAGE) was used to analytically solve combustion reactions. Different gasoline surrogates able to reproduce the chemical and physical properties of the gasoline used to gather the experimental data were tested; the results, in term of in-cylinder pressure trace and Heat Release Rate (HRR) shows a good agreements with the data measured at the engine test rig.
# Contents

Acronyms and symbols ........................................... xi

1 **Introduction** .................................................. 1
   1.1 GDI engines overview ...................................... 3
   1.2 Test case .................................................. 5

2 **Computational Fluid Dynamics Basics** ..................... 7
   2.1 Navier-Stokes equations ................................... 7
   2.2 Turbulent flows approximation ............................ 9

3 **Spray bomb** .................................................. 13
   3.1 Injector experimental characterization .................... 13
   3.2 Spray experimental characterization ....................... 14
   3.3 Grid settings .............................................. 16
   3.4 Simulation setup .......................................... 16
      3.4.1 Setup overview ....................................... 16
      3.4.2 Injection parameters evaluation ...................... 19
      3.4.3 Kelvin-Helmholtz and Rayleigh-Taylor models ....... 22
   3.5 Spray calibration .......................................... 25
      3.5.1 Grid sensitivity analysis ............................ 25
      3.5.2 Discharge coefficient sensitivity analysis .......... 31
      3.5.3 Rosin-Rammler SMD sensitivity analysis ............ 32
      3.5.4 RT time constant sensitivity analysis .............. 34
   3.6 Results .................................................. 36

4 **Cold cycle simulation** ..................................... 41
   4.1 Engine configuration and operating condition ............ 41
   4.2 Simulation setup .......................................... 42
      4.2.1 Surface preparation ................................... 42
      4.2.2 Boundaries, regions and initialization ............. 44
      4.2.3 Spray rate and orientation .......................... 52
      4.2.4 Grid control .......................................... 53
      4.2.5 Summary ............................................... 55
   4.3 Cold cycle results ........................................ 57
      4.3.1 Cylinder trapped mass ................................ 57
      4.3.2 Cylinder thermodynamic conditions ................. 58
      4.3.3 In-cylinder motion ................................... 61
      4.3.4 Spray orientation and distribution ................. 65
5 Combustion simulation

5.1 Combustion model

5.1.1 SAGE Detailed Chemical Kinetics solver

5.1.2 Toluene reference fuel

5.2 Combustion simulation setup

5.2.1 Source modelling

5.2.2 Combustion setup

5.3 Firing cycle results

5.3.1 Equivalence ratio

5.3.2 Flame front development

6 Conclusions and future work
List of Figures

1.1 Comparison of global \( CO_2 \) regulations for new passenger cars ............. 1
1.2 Classification of the GDI combustion systems, [15] ................................. 3
1.3 Operational modes of a DISI engine, [17] .............................................. 4
1.4 Engine torque as a function of engine speed ........................................... 6
2.1 Kinetic energy spectrum ............................................................................ 10
3.1 Injection profile: single nozzle mass flow rate as function of injection time for
an injection pressure of 100 bar ................................................................. 14
3.2 Spray orientation ....................................................................................... 15
3.3 Experimental LLP: (a) 01 test condition, (b) 02 test condition ................. 15
3.4 Spray morphology at 1 ms in 01 test condition: (a) rot 180, (b) rot 270 ....... 16
3.5 Computational domain grid refinement: side of the cell of 4.0 mm (black),
2.0 mm (green), 1.0 mm (red) and 0.5 mm (cyan) ........................................ 17
3.6 Spray orientation in Converge virtual environment: (a) rot 180, (b) rot 270,
(c) top view ......................................................................................... 17
3.7 Converge CSL_Gasoline_v1 and i-octane properties comparison: (a) density,
(b) saturation pressure, (c) surface tension and (d) viscosity as a function of
temperature ............................................................................................ 20
3.8 Injection profile: single nozzle mass flow rate as function of injection time for
the two tested injection pressure of 100 and 160 bar ................................... 21
3.9 Local grid refinements: (a) fixed embedding applied in a cylindrical volume,
(b) fixed embeddings applied in a truncated cone volume. Side of the cell of
4.0 mm equal to the base grid (black), 2.0 mm (green, embedding level equal
to 1), 1.0 mm (red, embedding level equal to 2) and 0.5 mm (cyan, embedding
level equal to 3) ...................................................................................... 26
3.10 LLP as a function of injection time for three different grid refinements: (a)
01 test condition rot180, (b) 01 test condition rot270, (c) 02 test condition
rot180 and (d) 02 test condition rot270 ...................................................... 28
3.11 Spray morphology obtained with GRID 2 (a), (b) and (c) and with GRID 3
(d), (e) and (f) respectively at 0.05 ms, 0.10 ms and 0.15 ms. ....................... 29
3.12 Grid after 2 ms in the middle plane of the domain with GRID 2 (a) and with
GRID 3 (b) ............................................................................................ 29
3.13 Number of cells as a function of the simulation time .................................. 30
3.14 LLP as a function of injection time for four \( C_d \): (a) 01 test condition rot180,
(b) 01 test condition rot270, (c) 02 test condition rot180 and (d) 02 test
condition rot270 ...................................................................................... 31
3.15 LLP as a function of injection time for four R-R characteristic SMD: (a) 01 test condition rot180, (b) 01 test condition rot270, (c) 02 test condition rot180 and (d) 02 test condition rot270. 32

3.16 Parcels velocity magnitude as a function of time measured on the plane 50 mm far from the injector tip for four R-R characteristic SMD: 01 test condition (a) and 02 test condition (b). 33

3.17 SMD as a function of time measured on the plane 50 mm far from the injector tip for four R-R characteristic SMD: (a) 01 test condition and (b) 02 test condition. 33

3.18 01 test condition: LLP as a function of time for five values of \( C_0 \): (a) rot180 and (b) rot270. 34

3.19 01 test condition: SMD as a function of time measured on the plane 50 mm far from the injector tip for five values of \( C_0 \). 34

3.20 02 test condition: LLP as a function of time for five values of \( C_0 \): (a) rot180 and (b) rot270. 35

3.21 02 test condition: SMD as a function of time measured on the plane 50 mm far from the injector tip for five values of \( C_0 \). 35

3.22 01 test condition: (a) LLP rot180, (b) LLP rot270, (c) SMD (d) droplet velocity magnitude on the plane 50 mm far from the injector tip. 37

3.23 02 test condition: (a) LLP rot180, (b) LLP rot270, (c) SMD (d) droplet velocity magnitude on the plane 50 mm far from the injector tip. 37

3.24 01 test condition: spray morphology at 0.4 (a), 0.6 (b), 0.8 (c), 1.0 (d), 1.2 (e), 1.4 (f), 1.6 (g) and 1.8 (h) ms in configuration rot180 and rot270. 38

3.25 02 test condition: spray morphology at 0.4 (a), 0.6 (b), 0.8 (c), 1.0 (d), 1.2 (e), 1.4 (f), 1.6 (g) and 1.8 (h) ms in configuration rot180 and rot270. 38

4.1 Engine geometry input data: (a) frontal view, (b) top view. 43

4.2 Geometry liner modifications: (a) and (c) initial configurations, (b) and (d) final configurations. 44

4.3 Intake valve geometry modifications: (a) and (b) initial configurations, (c) and (d) final configurations, with virtual disconnected triangles highlighted in green. 45

4.4 (a) intake valve, (b) exhaust valve. 47

4.5 Intake and exhaust valve lift profile as a function of crank angle. 47

4.6 Piston motion: distance of the piston crown from the BDC position. 48

4.7 (a) inflow boundary (brown), (b) outflow boundary (yellow). 49

4.8 Boundary conditions as a function of crank angle: (a) total intake pressure, (b) total intake temperature, (c) static exhaust pressure and (d) static exhaust temperature. 50

4.9 Geometry regions: blue intake system, red exhaust system and green cylinder. 52

4.10 Injection rate for an injection pressure of 200 bar as a function of the injection time. 53

4.11 Injection orientation: (a) frontal view, (b) lateral view, (c) view perpendicular to the injector \( z \) axis (26° titled with respect the horizontal plane). 54

4.12 Engine simulation embeddings: (a) frontal view, (b) lateral view. 54

4.13 Intake and exhaust valves lift and injection profile as a function of the crank angle. 54

4.14 Cold cycle exhaust mass flow and exhaust valves lift profile as a function of crank angle. 55
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.15</td>
<td>Cold cycle intake mass flow and intake valves lift profile as a function of the crank angle</td>
<td>57</td>
</tr>
<tr>
<td>4.16</td>
<td>Cold cycle intake mass flow rate, focus on the opening and closing phases</td>
<td>58</td>
</tr>
<tr>
<td>4.17</td>
<td>Cold cycle trapped mass as a function of the crank angle</td>
<td>58</td>
</tr>
<tr>
<td>4.18</td>
<td>Cold cycle cylinder pressure as a function of the crank angle</td>
<td>59</td>
</tr>
<tr>
<td>4.19</td>
<td>Cold cycle logarithmic Clapeyron diagram</td>
<td>59</td>
</tr>
<tr>
<td>4.20</td>
<td>Cold cycle cylinder temperature as a function of the crank angle</td>
<td>60</td>
</tr>
<tr>
<td>4.21</td>
<td>Rotation axes used for defining normal (blue) and cross tumble (red) and swirl (green)</td>
<td>61</td>
</tr>
<tr>
<td>4.22</td>
<td>Cold cycle cylinder tumble and turbulence intensity as a function of the crank angle</td>
<td>62</td>
</tr>
<tr>
<td>4.23</td>
<td>Cylinder flow field on the plane passing through the intake valve axis: 410 °CA (a), 450 °CA (b), 530 °CA (c), 640 °CA (d) and 410 °CA (e)</td>
<td>63</td>
</tr>
<tr>
<td>4.24</td>
<td>Comparison of the turbulent kinetic energy averaged over the cylinder and over the monitor point</td>
<td>64</td>
</tr>
<tr>
<td>4.25</td>
<td>Turbulent kinetic energy at spark timing (705 °CA) on the tumble plane passing through the cylinder axis (a), on the swirl plane passing through spark plug gap</td>
<td>65</td>
</tr>
<tr>
<td>4.26</td>
<td>Spray morphology at 480 °CA: (a) frontal view, (b) lateral view, (c) view perpendicular to the injector axis without the head, liner and exhaust valves</td>
<td>65</td>
</tr>
<tr>
<td>4.27</td>
<td>Intake valve face (a) and angle (b) liquid film results</td>
<td>66</td>
</tr>
<tr>
<td>4.28</td>
<td>Spray interaction with in-cylinder air motion on the tumble plane passing through the cylinder axis: 390 °CA (a), 440 °CA (b), 490 °CA (c) and 530 °CA (d); velocity magnitude color map</td>
<td>67</td>
</tr>
<tr>
<td>4.29</td>
<td>Instantaneous, cumulative and net mass on the liner (a) and piston crown (b)</td>
<td>67</td>
</tr>
<tr>
<td>5.1</td>
<td>Positive interaction (a), no interaction (b) and negative interaction (c) between two species</td>
<td>75</td>
</tr>
<tr>
<td>5.2</td>
<td>Example of a voltage curve during a spark event, [61]</td>
<td>76</td>
</tr>
<tr>
<td>5.3</td>
<td>Energy sources location</td>
<td>77</td>
</tr>
<tr>
<td>5.4</td>
<td>Cylinder pressure as a function of the crank angle for Blend 1, Blend 2 and Blend 3</td>
<td>79</td>
</tr>
<tr>
<td>5.5</td>
<td>Heat Release Rate as a function of the crank angle for Blend 1, Blend 2 and Blend 3</td>
<td>79</td>
</tr>
<tr>
<td>5.6</td>
<td>Cylinder pressure as a function of the crank angle for Blend 3 and Blend 4</td>
<td>80</td>
</tr>
<tr>
<td>5.7</td>
<td>Heat Release Rate as a function of the crank angle for Blend 3 and Blend 4</td>
<td>81</td>
</tr>
<tr>
<td>5.8</td>
<td>Equivalence ratio at spark timing (705 CA) on the tumble plane passing through the cylinder axis (a), on the swirl plane passing through spark plug gap (b)</td>
<td>82</td>
</tr>
<tr>
<td>5.9</td>
<td>Mass fraction as a function of the equivalence ratio binned in 20 intervals, from 0.0-0.1 to 1.9-2.0</td>
<td>82</td>
</tr>
<tr>
<td>5.10</td>
<td>Turbulent kinetic energy and velocity vectors at spark timing (705 °CA) on the tumble plane passing through the cylinder axis</td>
<td>83</td>
</tr>
<tr>
<td>5.11</td>
<td>In-cylinder temperature on the tumble plane passing through the cylinder axis (left column), on the swirl plane passing through the squish plane (right column). Sampling time: 5 °CA after SOC (a) and (b), 25 °CA after SOC (c) and (d), 45 °CA after SOC (e) and (f)</td>
<td>84</td>
</tr>
</tbody>
</table>
# List of Tables

1.1 F154 CB compression ratio, displacement and geometric features ............... 5  
1.2 Test case working point ........................................................................... 5  
3.1 Experimental test conditions used for spray calibration .............................. 13  
3.2 Injector characteristics and test conditions .................................................. 14  
3.3 Rosin-Rammler initial distribution parameters ............................................. 18  
3.4 Sub-models employed for the spray modeling .............................................. 19  
3.5 *Converge* Gasoline surrogate composition ............................................... 19  
3.6 Initial values of injection parameters considered in the spray calibration procedure .................................................. 25  
3.7 Grid definition in term of base grid, embedding and AMR scale for the three grids tested in the grid sensitivity analysis ................................................ 27  
3.8 Calibrated Rosin-Rammler distribution parameters ........................................ 34  
3.9 Calibrated injection parameters .................................................................. 36  
4.1 F154 CB compression ratio, displacement and geometric features ............... 42  
4.2 Case setup boundaries and regions ......................................................... 46  
4.3 Intake valve opening and exhaust valve closing at 7000 rpm and 21 bar bmep 46  
4.4 Wall boundaries initialization temperatures ................................................... 48  
4.5 Inflow boundary condition species and respective mass fractions ................ 51  
4.6 Regions initialization values ...................................................................... 52  
5.1 Ferrari surrogate gasoline properties ......................................................... 72  
5.2 Composition of the surrogates injected fuel ................................................ 77  
5.3 Properties of the surrogates injected fuel .................................................... 78  
5.4 Composition of the fourth surrogate .......................................................... 80  
5.5 Properties of the fourth surrogate .............................................................. 80
## Acronyms and symbols

### Acronyms

<table>
<thead>
<tr>
<th>Acronym</th>
<th>Definition</th>
</tr>
</thead>
<tbody>
<tr>
<td>AFR</td>
<td>Air Fuel Ratio</td>
</tr>
<tr>
<td>AMR</td>
<td>Adaptive Mesh Refinement</td>
</tr>
<tr>
<td>BDC</td>
<td>Bottom Dead Center</td>
</tr>
<tr>
<td>BMEP</td>
<td>Brake Mean Effective Pressure</td>
</tr>
<tr>
<td>CA</td>
<td>Crank Angle</td>
</tr>
<tr>
<td>EVC</td>
<td>Exhaust Valve Closing</td>
</tr>
<tr>
<td>HRR</td>
<td>Heat Release Rate</td>
</tr>
<tr>
<td>ICE</td>
<td>Internal Combustion Engine</td>
</tr>
<tr>
<td>IVO</td>
<td>Intake Valve Opening</td>
</tr>
<tr>
<td>I-Octane</td>
<td>Iso-Octane</td>
</tr>
<tr>
<td>KH</td>
<td>Kelvin-Helmholtz</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>LHV</td>
<td>Lower Heating Value</td>
</tr>
<tr>
<td>LLP</td>
<td>Liquid Length Penetration</td>
</tr>
<tr>
<td>MPI</td>
<td>Multi-Point Injection</td>
</tr>
<tr>
<td>MON</td>
<td>Motor Octane Number</td>
</tr>
<tr>
<td>NTC</td>
<td>No Time Counter</td>
</tr>
<tr>
<td>N-Heptane</td>
<td>Normal-Heptane</td>
</tr>
<tr>
<td>OEM</td>
<td>Original Equipment Manufacturer</td>
</tr>
<tr>
<td>ON</td>
<td>Octane Number</td>
</tr>
<tr>
<td>PDA</td>
<td>Phase Doppler Anemometry</td>
</tr>
<tr>
<td>Acronym</td>
<td>Description</td>
</tr>
<tr>
<td>---------</td>
<td>-------------</td>
</tr>
<tr>
<td>PFI</td>
<td>Port Fuel Injection</td>
</tr>
<tr>
<td>PISO</td>
<td>Pressure Implicit with Splitting Operators</td>
</tr>
<tr>
<td>PM</td>
<td>Particulate Matter</td>
</tr>
<tr>
<td>PRF</td>
<td>Primary Reference Fuel</td>
</tr>
<tr>
<td>PSD</td>
<td>Power Spectral Density</td>
</tr>
<tr>
<td>RANS</td>
<td>Reynolds-Averaged Navier-Stokes</td>
</tr>
<tr>
<td>RNG</td>
<td>Renormalization Group</td>
</tr>
<tr>
<td>RON</td>
<td>Research Octane Number</td>
</tr>
<tr>
<td>R-R</td>
<td>Rosin-Rammler</td>
</tr>
<tr>
<td>RT</td>
<td>Rayleigh-Taylor</td>
</tr>
<tr>
<td>S</td>
<td>Sensitivity</td>
</tr>
<tr>
<td>SMD</td>
<td>Sauter Mean Diameter</td>
</tr>
<tr>
<td>SOI</td>
<td>Start of Injection</td>
</tr>
<tr>
<td>TDC</td>
<td>Top Dead Center</td>
</tr>
<tr>
<td>TKE</td>
<td>Turbulent Kinetic Energy</td>
</tr>
<tr>
<td>TRF</td>
<td>Toluene Reference Fuel</td>
</tr>
<tr>
<td>VLP</td>
<td>Vapor Length Penetration</td>
</tr>
<tr>
<td>UDF</td>
<td>User Defined Function</td>
</tr>
<tr>
<td>3-D</td>
<td>3-Dimensional</td>
</tr>
</tbody>
</table>

**Symbols**

- \( A \) \hspace{1em} Area
- \( B_0 \) \hspace{1em} Kelvin-Helmholtz model size constant
- \( B_1 \) \hspace{1em} Kelvin-Helmholtz model time constant
$C_0$ Rayleigh-Taylor model time constant
$C_1$ Rayleigh-Taylor model size constant
$C_d$ Discharge Coefficient
$d x_{base\,grid}$ Base Grid Size
$HC$ Unburned Hydrocarbons
$K_c$ Thermal Conductivity Coefficient
$m$ Mass
$N_2$ Nitrogen
$O_2$ Oxygen
$p$ Pressure
$q$ Mass flow rate
$r$ Radius
$Re$ Reynolds Number
$S$ Surface
$T$ Temperature
$t$ Time
$V$ Volume
$v$ Velocity
$We$ Weber Number
$\nu$ Kinematic viscosity
$\rho$ Density
$\sigma$ Surface tension
$\phi$ Equivalence ratio
Chapter 1

Introduction

In the last few years, the more and more stringent environmental regulations have forced Original Equipment Manufacturers (OME) to develop new spark ignition engine technologies, such as variable valve lift, turbocharging and gasoline direct injection (GDI) [1]. As reported in figure 1.1 from 2021, the European Union fleet-wide average emission target for new cars is 95 g CO₂/km, which corresponds to a fuel consumption of around 4.1 l/100 km of petrol or 3.6 l/100 km of diesel. To withstand this target, more efficient combustion processes are required, being fuel consumption directly linked to CO₂ emissions.

![Figure 1.1: Comparison of global CO₂ regulations for new passenger cars](image)

Spark ignition engines will continue to play a fundamental role in the passenger cars market, thanks to the many advantages they offer, such as their simplified aftertreatment system and the possibility of integration with hybrid powertrains [2], [3]. In GDI engines, the fuel is directly injected into the combustion chamber; this leads to a more precise control of the injection timing and of the fuel injected mass, resulting in a better control of the mixture formation and so, of the combustion processes. The adoption of the GDI technology improves not only fuel consumption and emission characteristics, but also performances [4]. However, with respect to a standard gasoline port fuel injection engine (PFI), a different design of the combustion chamber is required [5]; moreover, the in-cylinder injection leads to a reduced time available for fuel atomization and evaporation.
and thus, to an higher interaction between the liquid fuel and the cylinder surfaces, resulting in fuel deposits on the combustion chamber walls. If these fuel films don’t evaporate before combustion starts, they will be oxidated in heavily sooting diffusion flames, leading to high particulate matter (PM) emissions. For this reason, a greater control of some working characteristics, such as the in cylinder gas motion, injection and ignition phases is needed.

Spray pattern, injection law and pressure play a fundamental role in the mixture preparation process [6], [7] that in turn affects combustion processes and thus the overall engine performances [8]. Spray pattern refers to a wider set of parameter such as the injector location, the number of injector holes and the direction of each spray beam; the injection event can be performed through a single injection or through multiple injections; in [9] is show that the two mentioned strategies lead to completely different results especially in working points characterized by low speed, whereas, for higher engine speed, the spray evolution is mainly influenced by the injector properties and injection strategy. Therefore, being GDI performance influenced by an extremely high number of factors, an exhaustive experimental study would be unfeasible; furthermore, as reported in section 1.1, GDI engines have to be optimized for a wide range of working conditions, each of one characterized by different mixture preparation processes. For this reasons, Computational Fluid Dynamics (CFD) is gaining increasingly importance in the design and choice of the engine working parameters. Moreover, optimization through only bench testing is extremely expensive and time consuming indeed, and some variables can be difficult to be three-dimensionally measured on a real engine prototype. This methodological shift is aligned with what experts point out: engine manufacturers need to change from a test-first culture to an Analysis-Led Design Process in order to "... accelerate the market transformation to high-efficiency, clean power sources for transportation"[10].

Two of the most challenging tasks in CFD engine simulations, are the spray modelling and the chemical combustion kinetics. As the liquid jet interacts with the surrounding air, it is subjected to a wide set of phenomena such as primary and secondary breakup, collisions, coalescence, evaporation, and mixing that affect the quality of the mixture composition; in turn, the mixture composition influences the combustion efficiency and the pollutants formation. This is why, the first phase of the work consists in the spray calibration, i.e. the definition of the models and of their parameters that are capable to reproduce the most important spray features, such as the liquid length penetration (LLP) and the droplets dimension and velocity.

In [11], the Taylor Analogy Breakup (TAB), the Cascade Atomization and Drop Breakup (CAB) and the Kelvin-Helmholtz Rayleigh-Taylor (KH-RT) are tested and validated in terms of spray penetration, droplets diameter and speed. The KH-RT model results to be the oe with the better match with experimental results. An evolution of the classical KH-RT model is validated in [12]; in this study, the breakup length, i.e. the distance after the which the RT model can contribute to the breakup, is not considered in the model, but the model is modified so that RT instabilities affect all drops outside the liquid core of the jet. A similar breakup concept is used in [13], where the validated spray model is then used to carry out full-engine GDI engine simulations. In the mentioned work, the combustion is modelled through the kernel flame model when the ignition-kernel flame has a structure smaller than the average grid size in the computational domain, while the G-equation is used when the flame structure is bigger than the a characteristic flow length scale. However, to properly model combustion phenomena, including auto-ignition processes and emissions, the use of detailed chemistry is fundamental [14]. For what concerns the chemical combustion kinetics, the main obstacle to overcome is the
definition of the fuel properties. As a matter of fact, either diesel and gasoline fuels are complex mixtures of compounds whose chemistry composition cannot be fully replicated. For this reason, instead of the actual fuel, surrogates, i.e. blends made up of a restricted set of compounds, with specific characteristics such as the octane number, density and lower heating value, are used.

In such a context, the aim of this work is the development of the engine Ferrari GDI F154 CB numerical model, capable to reproduce the experimental pressure curve in a specific engine operating point. The thesis activity is entirely performed on the 3D-CFD software Converge (V2.4) and it is made up of two main parts; the first one consists in the numerical characterization of the spray bomb, i.e. of the features of the fuel spray injected in a quiescent constant volume cubic vessel over two different operating conditions. The second one, exploits the developed spray, to assess the capability of the model of reproducing the in-cylinder combustion process. Furthermore, given the importance of the in-cylinder air motion in the mixture preparation process, an analysis on the dominant charge motion and turbulence level is performed over a cold engine cycle.

1.1 GDI engines overview

Mixture preparation can be achieved following three basic techniques, outlined in figure 1.2. In wall-guided, the interaction between the vapour fuel and the spark plug is generated by the geometric features of the combustion chamber; in the air-guided the fuel is directed toward the spark plug by the air motion (i.e. tumble or swirl) inside the combustion chamber and in spray-guided the spray is directly targeted on the spark plug. The first two techniques belong to the wide-spacing configurations, since there exists a relatively large distance between the spark plug gap and the injector tip, while the spray-guided technique belongs to the narrow-spacing category, being combustion assured by the small distance between the spark plug and the injector tip.

Figure 1.2: Classification of the GDI combustion systems, [15]

Being the injection directly inside the cylinder, the reduced time for evaporation has to be counterbalanced by an higher injection pressure; for this reason, even if the first GDI engines prototypes date back to the middle of the 20th century, their actual application started in the ’90s, with the development of electronically controlled high pressure injection systems. In [16] is shown that the increase of the injection pressure makes the combustion more stable reducing the cycle-to-cycle variations and that the spray induced turbulences help in accelerating the initial phases of the combustion.

Thanks to the extremely precise control of the fuel supply, GDI engines are more flexible and able to efficiently work under different operating conditions. A standard example of
operational modes of a DISI engine is reported in figure 1.3, from [17].

![Figure 1.3: Operational modes of a DISI engine, [17]](image)

For low load, low speed working points, usually the injection is delayed in order to obtain a stratified charge, i.e. a non-homogeneous charge, stoichiometric near to the spark plug to promote combustion, and extremely lean far from it. In conventional PFI engines, in the amount of in-cylinder fuel is related to the admitted charge, the operations of the engine in the low load region are extremely inefficient, since an heavy throttling is required to obtain a close to stoichiometric mixture; this increases the engine pumping losses [18], reducing the efficiency. It’s important to notice that charge stratification strategy at low loads is not always exploited, since an overall lean combustion would require the use of specific aftertreatment systems to perform NOx reduction within an oxidizing environment.

For higher engine loads, the fuel is injected during the intake stroke to obtain a close to homogeneous mixture; in these operating conditions, the main advantage is provided by the charge cooling produced by the fuel evaporation inside the combustion chamber that allows to increase the compression ratio and the spark advance (SA) increasing the thermodynamic efficiency. Indeed, in PFI engines, a significant portion of this heat is provided by the valve on which the fuel jet will deposit, resulting in a higher mixture temperature. The reduction of in-cylinder temperature provides:

- volumetric efficiency increase of 5%-10% [19] with respect to conventional PFI engine which results in a 10% increase of the bmep [20]

- The temperature reduction at the end of the intake phase is magnified during the compression stroke following the formula 1.1

\[ T_2 = T_1 \cdot CR^m \]

This gives the possibility of increasing the compression ratio and the spark advance, making the thermodynamic cycle more efficient and avoiding abnormal combustions.

- better acceleration transient performances since the increase of the injected mass of fuel doesn’t deposit on the intake valves and port, but effectively contributes to the actual AFR, leading to a power increase

For these reasons, GDI engines are able to provide lower fuel consumption and higher power output than engines equipped with conventional port fuel injection (PFI) or multi-point injection (MPI) systems [21], [22].
1.2 Test case

The studied spray is injected by the 7-holes high-pressure solenoid injector BOSCH HDEV for two different injection pressures and two different air temperatures and pressures. A set of experimental penetration curves, SMD and average droplets velocity as function of the injection time obtained through PDA are used to validate the model. Moreover, the comparison with the simulation results is qualitatively performed basing on the spray morphology evaluated on two different planes. The developed 3D-CFD spray model constitutes the starting point for the simulation of the combustion process during the engine cycle. The engine under study is the Ferrari 8-cylinders, 3,9 litres turbocharged GDI F154 CB. It provides a maximum power of 675 cv at 8000 rpm and a maximum torque of 760 Nm at 3000 rpm. Mixture preparation is performed through air-guided technique; both the intake and the exhaust valves come with variable cam phasing. Bore and stroke are respectively of 86,5 and 83,0 mm and the compression ratio is equal to 9,4.

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Parameter value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression ratio</td>
<td>9,4</td>
</tr>
<tr>
<td>Displacement</td>
<td>3,902 l</td>
</tr>
<tr>
<td>Bore</td>
<td>86,5 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>83,0 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>142,5 mm</td>
</tr>
<tr>
<td>Crank offset</td>
<td>0,8 mm</td>
</tr>
</tbody>
</table>

Table 1.1: F154 CB compression ratio, displacement and geometric features

The engine point under study is characterized by 21 bar of bmep and 7000 rpm (table 1.2).

<table>
<thead>
<tr>
<th>Engine speed [rpm]</th>
<th>bmep</th>
</tr>
</thead>
<tbody>
<tr>
<td>7000</td>
<td>21 bar</td>
</tr>
</tbody>
</table>

Table 1.2: Test case working point

Figure 1.4 shows the homologated normalized torque as a function of the engine speed. Regarding the combustion simulation, two set of data are provided and used as reference:

- Thermodynamic data (temperature, pressure and heat release rate) and intake and exhaust mass flow rates gathered from a validated GT-Power model

- The experimental average pressure trace for each engine cylinder and the average of all the cylinders
Figure 1.4: Engine torque as a function of engine speed
Chapter 2
Computational Fluid Dynamics Basics

This chapter gives an overview of the theoretical concepts that constitute the fundamentals of Computational Fluid Dynamics. It is focused only on the main important aspects, and it doesn’t provide a complete view of a such vast topic: to this regard, there exists a wide literature about CFD to which refer (e.g. [23]).

2.1 Navier-Stokes equations

The Navier-Stokes equations are a set of partial differential equations that describe the flow evolution of a fluid. Regardless of the complexity of the fluid system under study, the application and solution of the mass, momentum and energy conservation laws, allows univocally determining the behaviour of the system. These fundamental relations are reported in equations 2.4, 2.6 and 2.8 in their integral formulation; starting from the differential formulation, the transport or Reynolds theorem is applied to express the extensive property as a function the corresponding intensive one. As result, the density \( \rho \) is used for the mass, the momentum per unit volume \( \rho u \) for the momentum and the specific energy \( e \) for the energy. Through the Reynolds theorem, extensive \( \Psi \) and intensive \( \psi \) properties are related by formula 2.1. Generally speaking,

\[
\frac{d}{dt} \int_V \psi dV = \int_V \left( \frac{d\psi}{dt} + \psi \nabla \cdot \mathbf{u} \right)
\]

where

- \( V \) is the control volume
- \( \mathbf{u} \) is the eulerian velocity vector
- \( \nabla \cdot \) is the divergence operator

Mass conservation principle states that the mass of fluid \( M \), belonging to an arbitrary volume \( V \) within the fluid field doesn’t change with the motion of \( V \); this postulate can be written mathematically as reported in formula 2.2.
\[ \frac{dm}{dt} = 0 \quad (2.2) \]

Applying the transport theorem, with the density \( \rho \) instead of \( \psi \), in absence of external mass sources, equation 2.2 can be rewritten as

\[ \int_V \frac{d\rho}{dt} dV + \rho \nabla \cdot \mathbf{u} = 0 \quad (2.3) \]

that becomes formula 2.4 by using the Gauss theorem

\[ \int_V \frac{\partial \rho}{\partial t} dV + \int_S \rho \mathbf{u} \cdot \mathbf{n} dS = 0 \quad (2.4) \]

The principle of the momentum conservation postulates that the total derivative of the momentum associated to the volume \( V \) is at any time equal to the resultant of the external forces applied to it.

\[ \frac{d}{dt} \int_V \rho \mathbf{u} dV = \int_V \rho f dV + \int_S \mathbf{F} dS \quad (2.5) \]

where

- \( f \) are the volume forces (e.g. gravity)
- \( \mathbf{F} \) are the surface forces

Applying the transport and the Gauss theorems to the first member of equation 2.5, it can be rewritten as

\[ \int_V \frac{\partial (\rho \mathbf{u})}{\partial t} dV + \int_S (\rho \mathbf{u}) \mathbf{u} \cdot \mathbf{n} dS = \int_V \rho f dV + \int_S \mathbf{F} dS \quad (2.6) \]

The principle of the total energy conservation is derived from the first principle of thermodynamics. Indicating with \( \delta L \) the work done by the external forces on the volume \( V \) and with \( \delta Q_c \) the heat transferred from the external environment to the volume \( V \), the first principle of thermodynamics is written as

\[ dE = \delta Q_c + \delta L \quad (2.7) \]

The symbol \( \delta \), referred to work and heat, is used instead of \( d \) to denote an inexact differential, i.e. a function that doesn’t depend only on the initial and end state of the system, but on the type of transformation considered. Performing the same steps of the previous two conservation laws, 2.7 becomes

\[ \int_V \frac{\partial (\rho c_v)}{\partial t} dV + \int_S \rho c_v \mathbf{u} \cdot \mathbf{n} dS = \int_V \rho \mathbf{f} \cdot \mathbf{u} dV + \int_S \mathbf{F} \cdot \mathbf{u} dS - \int_S q_c \cdot \mathbf{n} dS \quad (2.8) \]

where the term \( q_c \cdot \mathbf{n} dS \) is the flux of specific heat per unit mass that crosses the infinitesimal surface \( dS \) in the unit time \( dt \).

Applying the Fourier law, the last term of equation 2.8 can be written as

\[ \int_S q_c \cdot \mathbf{n} dS = - \int_S K_c \nabla T \cdot \mathbf{n} dS \quad (2.9) \]

where
• \( \nabla T \) is the temperature gradient
• \( K_c \) is the thermal conductivity coefficient

Equations 2.2, 2.5 and 2.8 constitute a system of fully coupled non-linear partial differential equation. The non-linearity of the problem, makes the complete numerical solution of difficult implementation because of the necessity of solving up to the smallest time and length scales (section 2.2).

### 2.2 Turbulent flows approximation

Any flow, for Reynolds number higher than a critical value becomes turbulent, that is that its field variables (e.g. velocity, density) statistically fluctuate around a mean value; thus a fluctuating field can be defined in terms of average and fluctuations about the average, respectively \( \bar{V}_i \) and \( v_i \) in equation 2.10

\[
V_i = \bar{V}_i + v_i \tag{2.10}
\]

Comparing different turbulent motions, different intensities and size patterns can be observed; turbulent eddies are characterized by spatial and time scales, i.e. by a characteristic length and duration or turnover. Two fundamental length scales can be defined: the integral length scale \( L \), and the Kolmogorov length scale \( \eta \). The former is defined as the length scale of the eddies conveying most of the kinetic energy, whereas the latter is defined as function of kinematic viscosity \( \nu \) and viscous dissipation \( \varepsilon \) and determines the size of the smallest eddies.

\[
\eta = \left( \frac{\nu^3}{\varepsilon} \right)^{1/4} \quad t_\eta = \left( \frac{\nu}{\varepsilon} \right)^{1/2} \quad u_\eta = \frac{\eta}{t_\eta} = (\eta\varepsilon)^{1/4} \tag{2.11}
\]

where \( \eta \) is the Kolmogorov length scale, \( t_\eta \) is the Kolmogorov time scale and \( u_\eta \) is the Kolmogorov velocity scale. Among the integral and the Kolmogorov scales, a wide spectrum of scales can be defined according to the eddy cascade hypothesis, by which energy of larger eddies is consumed at the small scales by viscous dissipation. Energy transfer rate to the smallest scales is related to the viscous dissipation \( \varepsilon \) by

\[
\frac{k}{\lambda_t} = \varepsilon \tag{2.12}
\]

In equation 2.12, \( k \) is the kinetic energy, equal to \( \frac{3}{2} u'^2 \) for homogeneous isotropic turbulences (\( u' \) is the turbulence intensity of the eddies belonging to the integral scale) and \( \lambda_t \) is the integral time scale. Replacing the kinetic energy definition in 2.12, equation 2.13 is obtained.

\[
\frac{u'^3}{L} \propto \varepsilon \propto \frac{u_\eta^3}{\eta} \tag{2.13}
\]

The so-called \( k^{-5/3} \) law is obtained defining the kinetic energy as the derivative of the squared of the turbulence intensity with respect to the wavenumber \( k \).
\[ E(k) = \frac{du'^2}{dk} \propto \varepsilon^{2/3} k^{-5/3} \] (2.14)

Figure 2.1: Kinetic energy spectrum

Through direct numerical simulations (DNS), turbulences can be resolved numerically; however, this approach requires to have a grid in the computational domain and a solver time step with the same order of magnitude of the smallest space and time scales (Kolmogorov scales). Kolmogorov scales are proportional to \( Re^{3/4} \) which means that for \( n \) mesh points in the domain, the number of arithmetic operations scales with \( n^3 Re^{9/4} \), making unfeasible the application of DNS in engine simulations, where the Reynolds number is in the range of \( 10^5-10^7 \) [23].

Hence, turbulent flows must be approximated to be solved in reasonable time with limited computational power. Different approximation levels can be adopted to model turbulent flows; the most known approaches are Large Eddy Simulation (LES) and Reynolds Averaged Navier Stockes (RANS). In LES, turbulent fluctuations are directly computed, but differently from the DNS, turbulences below the so called subgrid scale, whose characteristics are related to the user imposed mesh size, are modeled by semi-empirical laws. Instead, within the RANS approach turbulent fluctuations are averaged over the entire spectrum; this results in a reduced computational efforts at the expense of some features, such as the possibility
of catching cycle-to-cycle variability.
Figure 2.1 shows the kinetic energy spectrum of turbulence as a function of the wavenumber $k$, highlighting the solved scales in DNS, LES and RANS.
Chapter 3

Spray bomb

The first step of the activity aims to calibrate the spray through a suitable choice of the model parameters, such as the ones of the Rosin-Rammler (R-R) distributions and of the breakup models. The calibration is performed based on three model output variables that are the liquid length penetration (LLP), and the Sauter mean diameter (SMD) and droplets speed measured on a plane 50 mm far from the injector tip. While the first output is already present in the Converge output files (spray.out and spray_ecn.out), the latter two are not automatically evaluated and provided by the software; for this reason, an on-purpose user defined function (UDF) has been written and implemented in the code.

The test conditions used for the spray are defined in terms of fuel temperature and injection pressure and of the chamber air temperature and pressure as reported in Table 3.1.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>343,15</td>
<td>100</td>
<td>323,15</td>
<td>1</td>
</tr>
<tr>
<td>343,15</td>
<td>160</td>
<td>323,15</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 3.1: Experimental test conditions used for spray calibration

A calibration process carried on multiple test conditions increases the model robustness, allowing it to reach higher predictivity level on different engine operating points.

3.1 Injector experimental characterization

Spray experimental characterization is performed using a standard gasoline characterized by a density of 720 kg/m³.

The injector used for the experimental characterization of the spray is a BOSCH multihole, high-pressure injector with solenoidal actuation that belongs to the HDEV 5 generation. The nozzle nominal diameter is equal to 220 μm and the static mass flow rate is equal to 923,5 g/min, when a pressure of 100 bar is applied on the injector needle. These last two data are used in section 3.4.2 for the evaluation of the discharge coefficient.

For what concerns the spray simulation, an injection event featuring an energizing time (ET) of 3000 μs is considered; the hydraulic delay was fixed equal to the experimental one (25 μs).
The instantaneous mass flow rate referred to a single nozzle for an injection pressure of 100 bar (first of the two test conditions table 3.1) has been provided as function of time as shown in figure 3.1.

For this first stage of the work, the position of each spray origin is not defined, whereas the spray orientation is reported in figure 3.2.

### 3.2 Spray experimental characterization

Since the simulation results will be compared with the experimental tests in order to tune the model, the aim of this section is to explain and show the experimental data used for the spray calibration activity. As already said, the comparison between experimental and simulation results is performed looking at three spray parameters, that are:

- Liquid length penetration (LLP)
- Sauter mean diameter (SMD) on a plane 50 mm far from the injector tip
- Droplets velocity magnitude on a plane 50 mm far from the injector tip

While for the last two spray parameters, measured through PDA technique, the outcome for each set of experimental conditions consists in a single curve in function of the time, for the LLP there are two of them (figure 3.3). Indeed, spray penetration is evaluated both on
Figure 3.2: Spray orientation

the frontal plane (plane with the normal corresponding to the y axis in figure 3.2) and on the lateral plane (plane with the normal corresponding to the x-axis in Figure 3.2); from now on, the first LLP configuration will be defined as rot270 (figure 3.4b), while the second configuration as rot180 (figure 3.4a).

Figure 3.3: Experimental LLP: (a) 01 test condition, (b) 02 test condition

As reported in figure 3.3, LLP experimental data is characterized by a first phase in which the curve is monotonically increasing, while after approximately 2 ms it starts to stabilise at a constant value; this behaviour is due to the fact that after this temporal interval, the spray reaches the boundaries of the observation window, making further measurements meaningless. For this reason, the comparison between experimental and simulation LLP is performed over the first 2 ms after the electric start of injection (SOI).

Moreover, a morphological evolution of the spray throughout time (as the ones provided for illustrative purpose in Figure 3.4), both in rot270 and in rot180, is provided as input data too; these data will be used for a qualitative comparison during the calibration process.
3.3 Grid settings

The mesh definition of the simulation environment is a crucial element of the simulation setup since both the solution precision and the computational time depend on it. The initial grid resolution, on the base of which a grid sensitivity analysis is performed successively, is defined as follow:

- Base grid made up of 4 mm side cubic cells
- Mesh refinement defined as function of the distance from the plane where the injector tip lies:
  - 0.5 mm side cubic cells in the environment volume up to the plane at 100 mm from the injector tip
  - 1.0 mm side cubic cells in the environment volume from the plane at 100 mm from the injector tip to the plane at 150 mm
  - 2.0 mm side cubic cells in the environment volume from the plane at 150 mm from the injector tip to the plane at 200 mm
  - 4.0 mm side cubic cells in the environment volume from the plane at 200 mm from the injector tip to the plane at 250 mm

The computational domain, as above described, is reported in figure 3.5. It’s important to underline that the grid resolution above defined has not to be strictly reproduced in Converge virtual environment, but it should serve as starting point and guideline for the first developments of the model setup (e.g. minimum cell size).

3.4 Simulation setup

3.4.1 Setup overview

The first step carried on in the 3D software is the definition of the simulation environment that consists of a cube of side 0.5 meters. The faces of the cube belong to a single boundary, and the entire volume included in it is assigned to a single region. Boundaries and regions allow to initialize variables, such as temperature, pressure and species enclosed. The gas contained in the virtual environment is quiescent fresh air without any trace of water vapour ([O₂] = 23% and [N₂] = 77%), and its temperature is kept fixed at 323.15 K, while pressure
Figure 3.5: Computational domain grid refinement: side of the cell of 4.0 mm (black), 2.0 mm (green), 1.0 mm (red) and 0.5 mm (cyan)

varies on the base of the experimental condition modeled, as reported in table 3.1. Assuming a starting thermal equilibrium between air and the computational domain boundaries, boundary temperature is set equal to air temperature.

In the middle of the top face of the cube are positioned the 7 nozzles of the injector tip, whose orientation with respect to the global reference system is expressed in cartesian coordinates; its implementatio result is reported in figure 3.6.

Figure 3.6: Spray orientation in Converge virtual environment: (a) rot 180, (b) rot 270, (c) top view

As briefly mentioned in section 3.1, the origin of each single nozzle is not available for the spray calibration step of the work, but it is provided with the engine CAD for the ICE cycle simulation. For this reason, six of the seven holes are positioned on a circumference with a radius of 1 mm, while the last one (the cyan spray beam) is positioned in the middle of the circle both for symmetry reasons and also to avoid sprays interaction immediately at the nozzle exit.

As mentioned in section 2.2, an important aspect affecting simulation results is the choice of the turbulence model used to account for effects of turbulence on the momentum, energy and species transport fields. To correctly predict these effects without the use of a turbulence model, all the turbulence scales, up to the Kolmogorov scales should be resolved. This scale is defined as

\[ \eta = \left( \frac{\nu^3}{\varepsilon} \right)^{\frac{1}{4}} \]  

(3.1)

where

- \( \eta \) is the Kolmogorov scale
\( \nu \) is the kinematic viscosity

\( \varepsilon \) is the viscous dissipation

and in typical engine simulations it is in the order of magnitude of \( 10^{-6} \) to \( 10^{-5} \) meters, a range of values so small to require extremely high computational time. For this reason a DNS (Direct Numerical Simulation) model is not used, and a turbulence model is required. The most common type of turbulence model for ICE simulations is the Renormalization group (RNG) \( k - \varepsilon \) turbulence model [24]. This means that the smallest solved scale is approximately the integral length scale, that in typical engine simulations is in the range of \( 10^{-4} \) to \( 10^{-3} \) meters; these values are important to be kept in mind since a smaller grid resolution doesn’t improve solution accuracy. The set of Navier-Stokes equations is closed by the RNG \( k - \varepsilon \) turbulence model since it is considered more accurate than the standard \( k - \varepsilon \) [25].

Converge solves the transport equations using the Pressure Implicit with Splitting of Operators (PISO) because it offers some advantages including the possibility of being applied both for compressible and incompressible flow and the semi-implicit treatment of sources and sinks [26].

Since the first part of the work aims at replicate the experimental spray behaviour in the simulation environment, a correct implementation of the injection parameters coupled with the right choice of breakup, collision and evaporative models are fundamental in order to accurately reproduce all the processes to which the liquid jet exiting from the nozzle is subjected. In this case study, the size of the drops exiting the nozzle is defined according to the Rosin-Rammler distribution, whose cumulative form is expressed by the following relation

\[
R = 1 - e^{-\left(\frac{X}{X'}\right)^n}
\]

where

\( X \) is the particle size

\( X' \) is the characteristic particle size, i.e. the particle size corresponding to 0.632 cumulative distribution undersize [27]

\( n \) is the spread parameter

It can be seen that for a fixed value of the location parameter \( X' \), the width of the R-R power spectral density (PSD) decreases with increasing the value of \( n \) (spread parameter), while keeping fixed the spread parameter and increasing the characteristic particle size \( X' \), the average particle size is moved toward higher values. The initial values of the spread parameter \( n \) and of the location parameter \( X' \) (which in a spray simulation is represented by the SMD) are defined as reported in table 3.3. These parameters are tested and validated against experimental data during the calibration procedure.

<table>
<thead>
<tr>
<th>Spread parameter ( n )</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMD</td>
<td>18 ( \mu )m</td>
</tr>
</tbody>
</table>

Table 3.3: Rosin-Rammler initial distribution parameters

Also the value of the spray cone angle is given as input to the model and is equal to 28 deg \( (\alpha = 28 \text{ deg}) \). As the liquid jet starts to interact with the surrounding air, it is
broken in smaller particles (droplets) due to breakup phenomena, up to a maximum of 128000 parcels per nozzle. The model adopted is a combination of the Kelvin-Helmholtz (KH) and the Rayleigh-Taylor (RT) models without breakup length option. However, being these phenomena of primary importance in the spray calibration process, paragraph 3.4.3 is completely dedicated to the explanation of the basic concepts and implementation of these breakup models. The description of the collision mechanism that occurs among the particles resulting from the breakup process is entrusted to the No Time Counter (NTC) collision model; the preference of this model with respect to the O’Rourke collision model is due to the fact that, for the same average error, the computational time in the first case increases linearly with the number of parcels in the domain, while in the latter the increase is quadratic [28].

The liquid fuel mass fraction for calculating spray penetration is imposed equal to 0.95 (LLP_0.95); this means that the LLP provided in the output file describing spray properties such as the number and the speed of injected parcels, the LLP and SMD (i.e. spray.out) is equal to the distance from the nozzle origin up to the last parcel that makes up the 95% of the overall parcels in the domain. Data provided in spray.out can be integrated by VLP and LLP_0.90, LLP_0.97, LLP_0.99 defined in spray.ecn.out. The droplets evaporate in i-octane (IC8H18) through the use of the Frossling model [29] without boiling model, a correlation used to determine the time rate of change of droplet size, that has already been proved to be valid for modelling gasoline evaporation (e.g. [30]).

<table>
<thead>
<tr>
<th>Turbulence model</th>
<th>RANS RNG $k-\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Injection model</td>
<td>Rosin-Rammler</td>
</tr>
<tr>
<td>Breakup model</td>
<td>Modified KH-RT</td>
</tr>
<tr>
<td>Drop drag model</td>
<td>Dynamic drop drag</td>
</tr>
<tr>
<td>Collision model</td>
<td>NTC</td>
</tr>
<tr>
<td>Evaporation model</td>
<td>Frossling w/o boiling model</td>
</tr>
</tbody>
</table>

Table 3.4: Sub-models employed for the spray modeling

### 3.4.2 Injection parameters evaluation

In literature can be find many procedures that describe how to blend hydrocarbons to get gasoline fuels with specific density, research octane number (RON) and motor octane number (MON) (i.e. [31], [32]). In this work, the Converge standard gasoline CSI_Gasoline_v1 is used since it has a good match with the gasoline used for the experimental activities. The composition of the Converge CSI_Gasoline_v1 is reported in table 3.5.

<table>
<thead>
<tr>
<th>Species name</th>
<th>Volume fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Isooctane (IC8H18)</td>
<td>0.50</td>
</tr>
<tr>
<td>Decane (C10H22)</td>
<td>0.35</td>
</tr>
<tr>
<td>Pentane (C5H12)</td>
<td>0.10</td>
</tr>
<tr>
<td>Dodecane (C12H26)</td>
<td>0.05</td>
</tr>
</tbody>
</table>

Table 3.5: Converge Gasoline surrogate composition

The properties of this blend, such as density, viscosity, surface tension, latent heat of
vaporization, conductivity, specific heat and vapor pressure are defined as function of temperature, every 10-K intervals, over the range of 0K up to the critical temperature. The most important spray-related properties of the CSI_Gasoline_v1 are reported in the figure below (figure 3.7) and compared to the ones of the i-octane, the gaseous specie in which the liquid fuel evaporates.

![Figure 3.7: Converge CSI_Gasoline_v1 and i-octane properties comparison: (a) density, (b) saturation pressure, (c) surface tension and (d) viscosity as a function of temperature](image)

In this section are also reported the analytical steps performed in order to get some model input parameters. The discharge coefficient $C_d$ is an adimensional number that indicates the ratio between the actual and the ideal mass flow rate through a nozzle for a one-dimensional isentropic flow \[33\].

$$C_d = \frac{A_{eff}}{A_{geom}} \quad (3.3)$$

where $A_{eff}$ and $A_{geom}$ are the effective area and the geometrical area respectively. For a given injection rate profile, $C_d$ defines the injection pressure, and thus, the injection speed. The discharge coefficient can be computed analytically from the static mass flow rate experimentally evaluated; in particular, knowing the static mass flow rate $q_{stat}$ for a specified pressure differential $\Delta p$, the injection speed at the outlet section of the injector can be computed applying Bernoulli’s law

$$\Delta p + \frac{1}{2} \rho v_{inj}^2 = \text{const} \quad (3.4)$$
\[ v_{inj} = \sqrt{\frac{2\Delta p}{\rho}} \]  

(3.5)

Then, by relating the instantaneous mass flow rate to the discharge coefficient through Formula 3.6

\[ q_{stat} = \rho_{fuel}A_{nozzle}C_d v_{inj} \]  

(3.6)

the value of the discharge coefficient can be computed as

\[ C_d = \frac{q_{stat}}{\rho_{fuel}A_{nozzle}v_{inj}} \]  

(3.7)

Substituting in the above formula the data already defined in section 3.1, the discharge coefficient assumes a value equal to 0.503.

This value, if compared to the one most spread in literature of about 0.7 results to be below the average. However, it can be found technical papers about spray simulation of GDI injectors [34], in which, the discharge coefficient measurement process leads to values not too far from the one computed here. Moreover, in order to dispel any doubts about the validity of the computed \( C_d \) value, a sensitivity study (section 3.5.2) is dedicated to the discharge coefficient sensitivity analysis.

As stated in section 3, there are two different sets of test conditions whose data are given in order to better capture the model predictivity. The discharge coefficient, in the presence of cavitation can vary with the injection pressure ([34]); however, being these variations almost negligible, they are neglected and the discharge coefficient is kept constant.

The mass flow changes with the injection pressure; not having EMI-like curves, that provide the injected quantity as a function of the ET for different injection pressures, the fuel mass flow rate measured at 100 bar is scaled by the square root of the ratio of the two different tested injection pressure in order to get the fuel mass flow rate at 160 bar as shown in Formula 3.8.

\[ q_{160 \text{ bar}} = q_{100 \text{ bar}} \sqrt{\frac{160}{100}} \]  

(3.8)

In this way, the mass flow rate for at 160 bar \( q_{160} \) is computed and reported is figure 3.8.

Figure 3.8: Injection profile: single nozzle mass flow rate as function of injection time for the two tested injection pressure of 100 and 160 bar
At this point, knowing the fuel mass flow rate for each of the two test conditions and assuming an instantaneous end of injection, it is possible to evaluate the total mass of fuel injected through a simple numerical integration of the mass flow rate over the time variable; the injected mass results equal to $4.586 \cdot 10^{-5} \text{kg}$ and to $5.801 \cdot 10^{-5} \text{kg}$ for the first and the second test condition respectively.

### 3.4.3 Kelvin-Helmholtz and Rayleigh-Taylor models

Atomization is one of the most significant aspects affecting spray behaviour; its importance is magnified in ICE simulations, since it's well known that injector performance heavily affects engine operation. Atomization cannot be directly solved by the CFD code since it would require a computational grid refinement and simulation time steps with the same order of magnitude of the length and time scale of the atomization process. For this reason, atomization is modeled as a sub-grid-scale process, with the consequence of introducing some empiricism in the computations [35].

The fuel leaves the injector as a continuous liquid phase, that impacting on the gas disintegrates in smaller droplets; more precisely, the liquid breakup process can be divided in primary breakup, in the region located close to the outlet section of the nozzle that leads to the formation of relatively large droplets, and in secondary breakup; here, the droplets resulted from the primary breakup are broken into smaller droplets ([36]). The atomization process is the result of the competition between surface tension, that tends to keep the liquid into a spherical shape [37], and internal and external forces generated by aerodynamic drag between liquid phase and gas phase, turbulence and implosion of cavitation bubbles, that instead promote the disruption process. On the base of injection parameters such as the liquid-gas relative velocity, the gas density and the liquid viscosity and surface tension, different breakup regimes can be identified.

**Converge** gives the possibility to chose among many different breakup models, including Kelvin-Helmholtz, Rayleigh-Taylor, Linearized Instability Sheet Atomization and Taylor Analogy Breakup. Among all the possible solutions, one of the most common found in literature and most appropriate for this kind of simulation involves the use of the Kelvin-Helmholtz model coupled with the Rayleigh-Taylor model, since the use of the KH-RT hybrid breakup model results in "... significantly reduced mesh and time-step dependency of the breakup model compared to simulations that do not use this approach" ([13]). More precisely a modified KH-RT model has been used in order to get more accurate simulation results compared to the experimental ones; the reasons of this choice are reported here below, after a description of the main important theoretical aspects of the two models. Both these models address the breakup phenomena to the growth of waves instabilities on the jet surface, but they differ in the mechanism that leads to their formation.

**KH BREAKUP MODEL**

Jet stability is described in detail by Reitz and Bracco [38]; a short summary of the model used is reported in the following.

The KH analysis is performed considering a cylindrical liquid jet of radius $a$ that penetrates a stationary incompressible gaseous environment. The analysis starts imposing on the cylindrical surface a number of infinitesimal perturbations with initial amplitude $\eta_0$ and a spectrum of wave numbers $k$. As the liquid jet and the gas interact, their amplitude
exponentially grows following the relation

$$\eta(t) = R(\eta_0 e^{ikx + \omega t})$$  \hspace{1cm} (3.9)$$

The growing perturbations are physically superimposed, but only the fastest growing perturbation with growth rate $\Omega_{KH}$ and correspondign wavelength $\Lambda_{KH}$, whose formulations as function of Weber, Reynolds, Taylor and Ohnesorge numbers is reported in equations 3.10 and 3.11, leads to breakup.

$$\frac{\Lambda_{KH}}{a} = 9.02 \frac{(1 + 0.45 Z^{0.5})(1 + 0.4 T^{0.7})}{(1 + 0.87 W e_g^{1.07})}$$  \hspace{1cm} (3.10)$$

$$\Omega_{KH} \left( \frac{\rho a^3}{\sigma} \right)^{0.5} = \frac{0.34 + 0.38 W e_g^{1.5}}{(1 + Z)(1 + 1.4 T^{0.6})}$$  \hspace{1cm} (3.11)$$

where:

- $Z = \left( \frac{W e_l}{R e_l} \right)^{0.5}$ is the Ohensorge Number
- $T = Z W e_g^{0.5}$ is the Taylor Number
- $W e_l = \frac{\rho U^2 a}{\sigma}$ is the Weber liquid Number and $W e_g = \frac{\rho_g U^2 a}{\sigma}$ is the Weber gas Number
- $R e_l = \frac{U a}{\nu_l}$ is the Reynolds number
- $a$ is the droplet radius
- $\rho_l$ is the liquid density and $\rho_g$ is the gas density
- $U$ is the liquid-gas relative velocity
- $\sigma$ is the droplet surface tension
- $\nu_l$ is the liquid kinematic viscosity

Parcels exiting the nozzle that have still not undergone to breakup phenomena are called parent parcels and are characterized by a radius $r_p$, defined according to the R-R-distribution. Knowing the value of the wavelength $\Lambda_{KH}$ corresponding to the maximum growth rate $\Omega_{KH}$, the radius of the parcels after breakup (i.e. the radius of the child parcel $r_c$) is defined as reported in equation 3.12

$$r_c = B_0 \Lambda_{KH}$$  \hspace{1cm} (3.12)$$

and the number of child parcels is defined according to the mass conservation principle. In equation 3.12, $B_0$ is called breakup size constant and is set equal to 0.6 [35]. From the same formula, the rate of change of the parent parcel can be evaluated as reported in equation 3.13

$$\frac{dr_p}{dt} = -\frac{r_p - r_c}{\tau_{KH}}$$  \hspace{1cm} (3.13)$$

where $\tau_{KH}$ is the breakup time (i.e. the time required by the perturbation to grow up to the breakage) and is defined by the equation 3.14

$$\tau_{KH} = \frac{3.726 B_1 r_p}{\Lambda_{KH} \Omega_{KH}}$$  \hspace{1cm} (3.14)$$
While \( B_0 \) doesn’t require to be calibrated, since its value of 0.6 is recognized as the most appropriate for engine spray simulation, the value of the parameter \( B_1 \), called breakup time constant, is initially imposed equal to 7, as suggested by the software for GDI simulation, but it could be subjected to calibration to obtain a better match with the experimental values. As it can be seen by the hereinabove expressions, an increase of the breakup time constant \( B_1 \) leads to breakup delay, whereas a reduction of it promotes breakup phenomena.

**RT BREAKUP MODEL**

Rayleigh-Taylor examines the stability of a liquid surface accelerated in a normal direction to the liquid-gas interface; RT breakup instabilities are generated when density gradient and parcel acceleration point opposite directions; this phenomenon is the one that commonly characterizes the trailing edge of the liquid droplets decelerated by drag forces [39]. As it happens in the KH model, also in the RT model, frequency and wavelength of the fastest growing waves are defined (equations 3.15, 3.16).

\[
\Lambda_{RT} = 2\pi \sqrt{\frac{3\sigma}{|F| (\rho_l - \rho_g)}}
\]  

\[
\Omega_{RT} = \sqrt{\frac{2 |F|}{3 \left[ \frac{|F| (\rho_l - \rho_g)}{3\sigma} \right]^{1/4}}}
\]  

In equation 3.15 and 3.16, \( |F| \) is the acceleration of a droplet subjected to drag forces, evaluated as reported in equation 3.17

\[
|F| = \frac{3}{8} C_D \frac{\rho_g v^2_{rel}}{\rho_l r}
\]  

If the wavelength corresponding to the fastest growth rate is smaller than the droplet diameter, instability waves begin to grow on the drop surface. The growth time is tracked, and if it is shorter than the breakup time, defined as reported in equation 3.18, the drop is assumed to breakup.

\[
\tau_{RT} = \frac{C_0}{\Omega_{RT}}
\]  

In equation 3.18 \( C_0 \) is a model parameter called RT time constant, usually imposed equal to unity [40].

Then, the radii of the new droplets is calculated as shown in equation 3.19

\[
r_e = \frac{2\pi C_1}{K_{RT}}
\]  

where \( C_1 \) is the RT size constant and \( K_{RT} \) is the wave number corresponding to the fastest growing perturbation. Actually, the model described here above is the inviscid form of the RT model. Converge instead is provided of the RT model extended in order to include viscosity, since it can have large effect in presence of large decelerations as it typically happens when dealing with high pressure injection phenomena [26].

**MODIFIED KH-RT MODEL**

The two breakup models mentioned above, if implemented in a competing manner, i.e. the model that predicts the shorter breakup time is the one responsible for the droplet break, lead to unrealistic predictions, since near the nozzle exit, where the aerodynamic drag forces
are predominant, the RT model is the governing mechanism that would predict too fast breakup phenomena. This is the reason why in the model setup, the option Create child particles in the KH-model menu is enabled; this option allows to separate the mechanism responsible of the primary breakup by the one responsible of the secondary. In particular, breakup of the injected liquid blobs (parent drops) is addressed only to KH instabilities, while the competition between the KH and RT mechanisms models the secondary breakup of parent drops into child drops.

3.5 Spray calibration

Model calibration consists in choosing the right model parameters that allows to fit the experimental results with the simulation ones. This is done through an iterative procedure made up of a series of sensitivity analysis, performed with the aim of studying how the model input parameters affect the results and which is the blend that provide results closer to reality. In particular, the calibration activity can be divided in the following two macro categories:

- Grid sensitivity analysis
- Injection parameters sensitivity analysis

In this study, the injection parameters sensitivity analysis is focused on the study of the effects generated on the simulation results by the discharge coefficient $C_d$, the R-R distribution and the breakup model parameters. Some of these values (e.g. $n$ and $X'$ of the R-R distribution) are provided as input data, others, such as the discharge coefficient is analytically evaluated and reported in section 3.4.2, while the KH-RT model parameters are set, as first choice, as the software suggests for simulating GDI. All these values are summarized in the table below (Table 3.6).

<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Parameter value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discharge coefficient</td>
<td>0.503</td>
</tr>
<tr>
<td>R-R spread parameter</td>
<td>5</td>
</tr>
<tr>
<td>R-R characteristic value</td>
<td>$18 , \mu m$</td>
</tr>
<tr>
<td>$B_0$</td>
<td>0.6</td>
</tr>
<tr>
<td>$B_1$</td>
<td>7</td>
</tr>
<tr>
<td>$C_0$</td>
<td>1</td>
</tr>
<tr>
<td>$C_1$</td>
<td>0.6</td>
</tr>
</tbody>
</table>

Table 3.6: Initial values of injection parameters considered in the spray calibration procedure

In the following paragraphs, only the most significant calibration phases are reported. As a matter of fact, the modification of some parameters leads to negligible results variation and for this reason they were not taken into account during the calibration procedure, preferring to keep the model with the value suggested by the software.

3.5.1 Grid sensitivity analysis

The goal of the sensitivity analysis is to find the grid convergent solution, i.e. the grid with the refinement level above which, a further refinement of the grid doesn’t lead to perceptible
outcomes variation. In this regard, the grid resolution reported in section 3.3 is used as starting point.

In *Converge*, the mesh is defined providing a value referred to the base grid (*Base grid size*), i.e. a value applied to the entire computational domain that indicates the dimension of the side of the cells in which the volume will be divided. Then, through the use of a tool called *Fixed embedding*, it is possible to locally refine the mesh. In this case, the user has to define three main parameters:

- application volume (e.g. a geometrical volume user-defined, the volume around a boundary or around an injector)
- activation time (e.g. permanent, cyclic)
- embedding scale: it is an integer number, positive to refine the mesh or negative to coarse it, that scales the base grid size on the base of the following relation

\[
\frac{dV_{\text{embedded}}}{dV_{\text{base grid}}} = \frac{dV_{\text{base grid}}}{2^{\text{embedding scale}}}
\]

To increase the grid refinement level, there is also the possibility of using the *AMR*, but this tool will be further described going on with the grid sensitivity analysis since the mesh adopted in the first simulation trials doesn’t require its application.

At a first glance, the grid proposed in section 3.3 doesn’t seem to be efficient, since there are many regions in which the mesh resolution is extremely high, even if they are far from the spray jet. Moreover, a faithful reproduction of that grid would lead to an extremely high number of cells, in the order of 215 millions. To mitigate this problem, a possible solution would be to reduce the mesh accuracy in the regions not affected by spray phenomena. Two possible solutions are reported in figure 3.9, in which the embedding activation volume is reduced first to a cylinder and then to a truncated cone.

![Figure 3.9: Local grid refinements: (a) fixed embedding applied in a cylindrical volume, (b) fixed embeddings applied in a truncated cone volume. Side of the cell of 4.0 mm equal to the base grid (black), 2.0 mm (green, embedding level equal to 1), 1.0 mm (red, embedding level equal to 2) and 0.5 mm (cyan, embedding level equal to 3)](image)

Despite this, the number of cells in the domain remains pretty high, about 60 millions (figure 3.9a) and 30 millions (figure 3.9b).
For this reason a number of changes have been done and three different grid configurations have been produced for the sensitivity analysis; from now on, they will be referred to as GRID 1, GRID 2 and GRID 3; the modifications brought to the model are summarized in the following bullet list:

- Increase of the base grid from 2.0 m to 16 mm: by analyzing the experimental data it can be seen that the spray LLP after 2 ms is in the order of 75 mm for both the test conditions (figure 3.3); this means that increasing the grid refinement above this value is irrelevant to the simulation results.

- Embeddings geometry as defined in figure 3.9b to avoid mesh refinement in areas not affected by the spray; their scale level remains the same (3,2,1) for GRID 2 and GRID 3, while it is increased of one level (4,3,2 respectively) in GRID 1. It’s important to underline the fact that, having changed the base size, even if the embeddings scale remains the same, the mesh results coarser. In GRID 2 and GRID 3 the embeddings lead to cubic cells with side of 2.0 mm, 4.0 mm and 8.0 mm, while 1.0 mm, 2.0 mm and 8.0 mm in GRID 1.

- The AMR is activated or disactivated on the base of the value assigned to the sub-grid criterion; if the difference between the actual and the resolved field is greater than the user-defined value, the cell is embedded. The maximum scale level is imposed equal to 5 to have the possibility of having the same maximum grid resolution of the initial model (0.5 mm). In order to avoid too large cells number, the maximum number of cells in the entire domain is imposed equal to 5 millions.

The AMR is activated for temperature and velocity fields, only in configurations 1 and 2, with an imposed sub-grid criterion of 0.5 m/s and 2.5 K respectively.

For sake of clarity, grid characteristics are summarized in Table 3.7.

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>GRID 1</td>
<td>16</td>
<td>4, 3, 2</td>
<td>5</td>
<td>0.5</td>
</tr>
<tr>
<td>GRID 2</td>
<td>16</td>
<td>3, 2, 1</td>
<td>5</td>
<td>0.5</td>
</tr>
<tr>
<td>GRID 3</td>
<td>16</td>
<td>3, 2, 1</td>
<td>no</td>
<td>2</td>
</tr>
</tbody>
</table>

Table 3.7: Grid definition in term of base grid, embedding and AMR scale for the three grids tested in the grid sensitivity analysis.

Figure 3.10 reports the LLP obtained for both test conditions without any calibration of the injection parameters. It can be seen that in every case the third grid, which is the coarser one, since it is without AMR, is not able to properly describe the spray behaviour. Instead, LLP obtained with the first and the second grid are almost coincident and already able to reproduce with a good approximation the first section of the experimental curve. The fact that there are negligible differences between the first two simulations is due to what already explained in paragraph 3.4.1: as a matter of fact, when performing a RANS simulation, a reduction of the dimension of the mesh below the scale that can be well approximated by the integral one doesn’t improve solution accuracy. For what concerns this aspect, it can be noted that the minimum cell size in the first and second simulation has the side of 0.5 mm, value that is near to the one mentioned in [24].
Figure 3.10: LLP as a function of injection time for three different grid refinements: (a) 01 test condition rot180, (b) 01 test condition rot270, (c) 02 test condition rot180 and (d) 02 test condition rot270

The importance of the AMR is well captured by the qualitative comparison of the spray morphology obtained in the simulation with AMR (GRID 2) and without AMR (GRID 3) (figure 3.11). It can be noted that the AMR allows to maintain a clear distinction between the different plumes exiting the nozzles, while without AMR this definition level cannot be captured.

Moreover, figure 3.12 allows to highlight the way the software performs the mesh operation: every cell is surrounded by other ones that differ for no more than one embedding level. This happens also when applying AMR, through the creation of a transition region (embedding level equal to 4) between the region in which the AMR reaches the maximum embedding level (embedding level equal to 5) and the region without it (embedding level equal to 3).

At this point, the choice between one of the first two grids is dictated by simulation time and memory required. Obviously, the second grid, providing results extremely close to the ones obtained through the third grid, with a lower number of cells in the computational domain, requires less computational efforts and for this reason is chosen to carry on with the work.
Figure 3.11: Spray morphology obtained with GRID 2 (a), (b) and (c) and with GRID 3 (d), (e) and (f) respectively at 0.05 ms, 0.10 ms and 0.15 ms.

Figure 3.12: Grid after 2 ms in the middle plane of the domain with GRID 2 (a) and with GRID 3 (b)
Figure 3.13: Number of cells as a function of the simulation time
3.5.2 Discharge coefficient sensitivity analysis

The next sensitivity analysis is performed on the value of the nozzle coefficient of discharge; its correct definition is fundamental since it defines the effective nozzle area, influencing spray velocity at the injector outlet section and thus all the phenomena that the liquid jet will be heading.

The value analytically computed, equal to 0.503, is well below the average one found in literature of 0.7; smaller values, can be sporadically reached overcome (up to 0.42 for GDI swirl injector [41]).

Thus, this analysis has been performed to check the validity of the computed value. Furthermore, the discharge coefficient can be evaluated only for the first test condition since the value of the static mass flow rate is provided only for that injection pressure (100 bar); through this analysis, it is possible to validate its worthiness also for the second injection pressure of 160 bar.

For both test conditions, 4 simulations with different discharge coefficients were performed, starting from the analytical one ($C_d = 0.503$) and increasing it to 0.6, 0.7, and 0.9. In this way, it is possible to clearly understand the effects of the discharge coefficient on the LLP.

From the above plots (figure 3.14), it can be seen that, as expected, by increasing the discharge of coefficient, the LLP is reduced. This is due to the velocity magnitude reduction generated by the increase of the effective nozzle discharge area. The best match with the experimental data is obtained using the discharge coefficient analytically evaluated both in the near and in the far field; for this reason, it has been decided to continue the calibration.

![Figure 3.14: LLP as a function of injection time for four $C_d$: (a) 01 test condition rot180, (b) 01 test condition rot270, (c) 02 test condition rot180 and (d) 02 test condition rot270](image-url)
activity with $C_d = 0.503$.

3.5.3 Rosin-Rammler SMD sensitivity analysis

At this point of the calibration procedure, the goal is to reduce the LLP in the far field. Looking at the SMD experimental values obtained on a plane 50 mm far from the injector tip it can be noted that they are almost equal to the one imposed in the R-R distribution characteristic SMD at the injector outlet. This seems to be in contrast with the physical spray evolution since the average SMD expected value after breakup phenomena should be smaller than the one before it. For these reasons the second option is chosen.

On the base of the concept just explained, simulations are carried on only with larger R-R characteristic SMD values than the one provided as input of 18 $\mu m$; in particular the values chosen are 27 $\mu m$, 36 $\mu m$ and 54 $\mu m$.

As in the previous calibration steps, LLP results are reported (figure 3.15) as function of time for both test conditions and in both configuration (rot 180 and rot 270).

It can be seen that increasing the value of the characteristic SMD the LLP is reduced in a non-linear way: the reduction of LLP is by far more evident between the two curves obtained with R-R characteristic SMD equal to 18 $\mu m$ and 27 $\mu m$ than between the ones obtained with 36 $\mu m$ and 54 $\mu m$.

Moreover, the effect of the R-R characteristic SMD is almost negligible in the near field,
while it becomes more noticeable as the spray moves forward into the domain. Figure 3.16 shows the droplet average speed as a function of the R-R characteristic SMD; it can be noted that, as the R-R characteristic SMD is increased, the average droplet velocity measured on the plane 50 mm far from the injector tip is reduced; also in this case the velocity reduction is not linear but, it’s more evident for small R-R characteristic SMD.

![Figure 3.16: Parcels velocity magnitude as a function of time measured on the plane 50 mm far from the injector tip for four R-R characteristic SMD: 01 test condition (a) and 02 test condition (b)](image)

Finally, the value of the SMD in the observation plane are plotted; from these graphs (figure 3.17) the following aspects can be highlighted:

- The increase of the R-R characteristic SMD value results in the increase of the SMD in the observation plane, as expected.
- The reduction of the LLP by increasing the R-R characteristic SMD value is shown by these plots too (figure 3.17). The vertical line is generated by the initialization value imposed in the UDF and defines the first instant in which the first parcel appears in the observation plane.

![Figure 3.17: SMD as a function of time measured on the plane 50 mm far from the injector tip for four R-R characteristic SMD: (a) 01 test condition and (b) 02 test condition](image)

On the base of the LLP, SMD and velocity magnitude results obtained, the calibration
proceeds with the R-R characteristic SMD equal to 27µm. Table 3.3 can be now updated with the values reported in Table 3.8.

<table>
<thead>
<tr>
<th>Spread parameter n</th>
<th>5</th>
</tr>
</thead>
<tbody>
<tr>
<td>SMD</td>
<td>27 µm</td>
</tr>
</tbody>
</table>

Table 3.8: Calibrated Rosin-Rammler distribution parameters

### 3.5.4 RT time constant sensitivity analysis

Through the previous calibration steps, the simulated LLP has reached a rather good fit with the experimental data. However, an attempt of reducing the difference between the model and the experimental SMD on the plane 50 mm far from the injector tip is still performed. For the same reasons explained in section 3.5.3, to avoid variations in the results in the near field, the choice is to modify RT parameters rather than the KH ones.

As reported in paragraph 3.4.3, the RT time constant $C_0$ is proportional to the RT breakup time (equation 3.18). The increase of its value leads to faster breakup phenomena, while its reduction vice versa. As reported in table 3.6, up to now calibration has been performed with $C_0 = 0.6$; for each test condition, the following RT time constant values are tested: $C_0 = 0.1$, $C_0 = 0.4$, $C_0 = 0.5$, $C_0 = 0.8$ and $C_0 = 1.0$.

In this section, differently from what done in the previous chapters about sensitivity analysis, the spray behaviour in the two test conditions is slightly different. This is why the two test conditions are analysed sequentially, first 01 test condition and then 02 test condition, rather than in parallel.

In the first test condition, values of $C_0$ in between 0.4 and 1.0 leads to negligible differences in the LLP curve (figure 3.18), while a substantial LLP increase is obtained with $C_0 = 0.1$. For what concerns the SMD values in the observation plane a similar trend is found; in fact a noticeable reduction in the SMD is obtained only with $C_0 = 0.1$ (figure 3.19).

Based on this results, the most appropriate $C_0$ value is 0.4 since it doesn’t reduce LLP prediction accuracy and at the same time provide better SMD values.

The same simulations are carried on for the second test condition and results are reported...
Figure 3.19: 01 test condition: SMD as a function of time measured on the plane 50 mm far from the injector tip for five values of $C_0$ below; to avoid having too many lines only the most significant are reported here.

Figure 3.20: 02 test condition: LLP as a function of time for five values of $C_0$: (a) rot180 and (b) rot270

Figure 3.21: 02 test condition: SMD as a function of time measured on the plane 50 mm far from the injector tip for five values of $C_0$
Differently from what happens in the first test condition, here even small reductions of the RT time constant (e.g. $C_0 = 0.4$) leads to a large LLP increase (figure 3.20) and the variation of the SMD is almost inversely proportional with the RT time constant (figure 3.21).

Thus, even if a small $C_0$ value reduction would have a positive effect in the SMD value in the first test condition, the choice is not to reduce it, since the drawbacks that this would lead in the second test condition would more than compensate the benefits obtained in the first test condition.

### 3.6 Results

A fundamental pre-requisite for realistic simulations of GDI engine cycle is an accurate prediction of spray formation. To ensure a better model predictivity the model parameters are tuned on the base of experimental data obtained in two different test conditions; to guarantee an adequate model robustness, the calibration procedure was performed using the same parameters for both the test conditions. The nozzle discharge coefficient of 0.503 analytically computed turned out to be correct. Spray model KH size and time constant are 0.6 and 7.0 respectively, while RT size and time constant are 0.6 and 1.0 respectively. Rosin-Rammler spread parameter is 5 and the distribution characteristic size is equal to 27 $\mu$m (table 3.9).

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Discharge coefficient $C_d$</td>
<td>0.503</td>
</tr>
<tr>
<td>KH size constant</td>
<td>0.6</td>
</tr>
<tr>
<td>KH time constant</td>
<td>7.0</td>
</tr>
<tr>
<td>RT size constant</td>
<td>0.6</td>
</tr>
<tr>
<td>RT time constant</td>
<td>1.0</td>
</tr>
<tr>
<td>Spread parameter $n$</td>
<td>5</td>
</tr>
<tr>
<td>SMD</td>
<td>27 $\mu$m</td>
</tr>
</tbody>
</table>

Table 3.9: Calibrated injection parameters

Spray penetration, droplet velocity and SMD on the plane 50 mm far from the injector tip were validated. Results are reported for the first (figure 3.22) and the second (figure 3.23) test conditions.

A good match of SMD and droplet velocity magnitude is obtained, except for SMD in the first test condition; here the simulated value is larger than the experimental one. However, taking due account that the model parameters must be able to replicate spray behaviour for both test conditions, and that a compromise must be find, the result can be considered acceptable. An extremely good match in the liquid penetration is obtained for both the injection pressures.

The goodness of these results is evident also from the spray morphological evaluation reported in figures 3.24 and 3.25.

The spray model validated in spray bomb simulation is used to perform the GDI engine simulations.
Figure 3.22: 01 test condition: (a) LLP rot180, (b) LLP rot270, (c) SMD (d) droplet velocity magnitude on the plane 50 mm far from the injector tip.
Figure 3.23: 02 test condition: (a) LLP rot180, (b) LLP rot270, (c) SMD (d) droplet velocity magnitude on the plane 50 mm far from the injector tip

Figure 3.24: 01 test condition: spray morphology at 0.4 (a), 0.6 (b), 0.8 (c), 1.0 (d), 1.2 (e), 1.4 (f), 1.6 (g) and 1.8 (h) ms in configuration rot180 and rot270
Figure 3.25: 02 test condition: spray morphology at 0.4 (a), 0.6 (b), 0.8 (c), 1.0 (d), 1.2 (e), 1.4 (f), 1.6 (g) and 1.8 (h) ms in configuration rot180 and rot270
Chapter 4

Cold cycle simulation

Now that the spray injection parameters are calibrated, the CFD simulation can be carried out on the entire engine cycle. Being massive the number of inputs data and parameters required by the software to perform this step, this phase of the work is divided in two parts: the first one with the aim of simulating the engine cycle without combustion (i.e. cold cycle), while in the second one will be considered the combustion processes, too. Doing in this way, is easier to distinguish whether a variance between the simulation results and the experimental ones is due to an error in the input files (e.g. valve phasing or boundary conditions) or to combustion related parameters. Moreover the convergence of the field variables requires some simulation time to be reached; for this reason, this simulation is performed to obtain a map.dat file, that is a file containing all the variables defined in each point of the computational domain, from which the firing cycle simulations will start. Thus, the cold cycle simulation has to be intended as an intermediate step through which is possible to check and validate the following aspects:

- Gas exchange process: intake and exhaust air mass flows, affected both by valve phasing and lift and by the imposed boundary conditions; these factors affect the amount of in-cylinder trapped mass, that consequently influences the cylinder pressure at firing time and the pressure trace in the complete engine cycle simulation.
- Turbulences and organized motions inside the combustion chamber
- Spray orientation and distribution: since spray distribution into the combustion chamber heavily affects combustion phenomena, it’s extremely important that the injector and its nozzle spray beams are correctly pointed.

4.1 Engine configuration and operating condition

The engine studied is the Ferrari F154 CB twin-turbocharged GDI V8 gasoline engine. The main important F154 geometrical parameters of the CB configuration, are summarized in table 4.1.

The operating condition for which the simulations are performed is an high speed, high load working point, that are respectively 7000 rpm and 21 bar of breaking mean effective pressure; in this operating point the measured air mass flow is equal to 1908 kg/h, and the gasoline mass flow is equal to 177.2 kg/h; the air-fuel equivalence ratio $\lambda$ is equal to 0.739,
<table>
<thead>
<tr>
<th>Parameter name</th>
<th>Parameter value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Compression ratio</td>
<td>9.4</td>
</tr>
<tr>
<td>Displacement</td>
<td>3.902 l</td>
</tr>
<tr>
<td>Bore</td>
<td>86.5 mm</td>
</tr>
<tr>
<td>Stroke</td>
<td>83.0 mm</td>
</tr>
<tr>
<td>Connecting rod length</td>
<td>142.5 mm</td>
</tr>
<tr>
<td>Crank offset</td>
<td>0.8 mm</td>
</tr>
</tbody>
</table>

Table 4.1: F154 CB compression ratio, displacement and geometric features

and the injection occurs early. These last two aspects are perfectly aligned with the injection strategy adopted at full load by OEMs; as a matter of fact, the adoption of this strategy allows to obtain a rich homogeneous charge; the evaporation of an amount of fuel larger than the stoichiometric one, has the effect of cooling the charge, increasing the volumetric efficiency, and thus performances on one hand, and decreasing the temperature of the mixture on the other hand; this last point, is particularly important, especially for turbocharged engines, since a temperature reduction could prolong the time to end-gas auto-ignition and finally suppress knock [42], [43].

Results validation is performed against two set of data: the first one, that includes either thermodynamic and mass flow data comes from a GT-Power model already validated, whereas the second one coming from experimental tests adds to the first set the in-cylinder pressure stress analysis.

4.2 Simulation setup

Before going into detail with the procedure followed to set up model some time parameters are defined here, to make easier the comprehension of the following paragraphs. The simulation start time is set 180 °CA after the TDC firing. This means that the simulation starts during the exhaust phase; this allows to dedicate the first simulation steps to the field variable stabilization process, making the domain ready to properly simulate the intake phase. The simulation lasts 720 °CA and the section of the cycle used to stabilize the variables is not repeated, since, in the simulation of a cycle without combustion, the in-cylinder pressure after TDC firing is lower than the one imposed in the exhaust boundary condition file, resulting in back flow from the exhaust port into the cylinder.

In this way, the simulation is centered on the intake phase and on the compression stroke, which are the actual object of study of the cold cycle simulation.

In the simulation the TDC firing occurs at 360 °CA; however, since the most diffused conventions used in engine cycle simulations defines the TDC firing at 720 °CA, cycle phases and results are reported translated of 360 °CA to be aligned with this norm.

4.2.1 Surface preparation

The internal combustion engine geometry must be provided to Converge as a triangulated surface; this means that it has to be exported or from a CAD program in .stl format or directly provided or in a properly formatted .dat file.
After having imported the ICE geometry, there are several tasks that the user could be required to perform in order to obtain a ready to use geometry; they can be summarized in the three following large items:

- **Repair defects in the geometry:** geometry defects are highlighted in the Diagnosis dock and can be divided in defects that prevent the Converge solver from running, classified as errors and others, classified as warnings, that could lead to solution inaccuracy. To the first class of defects belong the intersections, nonmanifold edges, normal orientation and open edges, whereas to the second overlapping triangles, aspect ratio, small area and small angle, whose threshold values are user-imposed.

- **Flag boundaries:** this task consists in splitting the surface in different areas, named boundaries and is performed to easily manipulate the geometry and to assign different boundary and initial conditions and other features to different boundaries.

- **Prepare piston and valves for motion:** when importing a surface geometry file, the piston and the valve stem may be misaligned with respect the liner and the valve motion respectively; since the motion of the piston and of the valve deforms the surface, everything must be aligned.

Moreover, two minor changes will be applied to the geometry to operate in a condition as close as possible to Converge best practice:

- **The liner must have a cylindrical surface, without any geometrical irregularity**

- **The valves, when in minimum lift configuration, i.e. when they are closed, have to be properly radially aligned with their seat in order to reduce issues related to a complex generation of the disconnected triangles, that are virtual triangles built to simulate the closed valve.**

After having briefly summarized the main tasks related to the geometry preparation, in the following is described item by item the procedure used in this work.

As already mentioned, since it’s warmly suggested to have the liner made up of a completely cylindrical surface, some modifications need to be made to pursue this goal; the areas of interest are the cylinder head in the region of the injector cave and the contact area between the liner and the piston bowl. Here, the triangles of the liner extend beyond the cylinder reaching the head and the piston; thus, it’s required to delete the triangles, and rebuild them in three different sections using the triangles creation tool (loft directionally option): then,
when the boundaries will be defined, the first one will be assigned to the piston crown, the second one to the cylinder head and the last one will be the liner as reported in figure 4.2.

Now that the geometry is almost complete, boundaries can be flagged. Section 4.2.2 is completely devoted to the description of the boundaries and to their initializations, but the concept is introduced here, since there are references to this topic in the last step of surface preparation herebelow. To perform this task, virtual borders on the surface geometry, called boundary fences, are created and then each area bounded by them is assigned to a boundary.

*Converge* doesn’t allow the intersection of surface triangles; thus, to simulate the closed valve, with the aim of avoiding leakages between the valve head and the valve seat, it creates disconnected triangles. It’s important that the disconnect triangles are as regular as possible. For this reason, the fillet that links the valve stem to the valve head is slightly modified with the aim of having a cylindrical disconnect surface. The red circumference in figure 4.3c is built centred with the valve stem axis and with the same radius of the valve seat. Then, the original triangles are deleted and built following the same procedure of the previous point.

Actually, this modification has to be performed after having set the minimum lift in the *Boundary* menu (0.2 mm for both intake and exhaust valves), since the translation of the valve with respect to its seat would change the axial positioning of the new triangles.

Finally, the geometry diagnosis tool is launched to look for possible geometry defects; if none of them is detected, the geometry is ready to be exported and the model setup can move forward.

### 4.2.2 Boundaries, regions and initialization

The division of the entire surface in different boundaries is performed for multiple reasons, concerning both geometry management, field variables initializations and constraints application (boundary conditions). With regard to this second category, it’s crucial to correctly define the location and the conditions of the boundary, since each boundary applies con-
straits to the partial differential transport equations, which in this way yield to a unique solution. Then the defined boundaries are grouped into regions, which are used to initialize and to connect or disconnect specific parts of the computational domain, such as intake and exhaust system with cylinder during intake and exhaust phase respectively. In table 4.2 are listed the boundaries defined in this case setup and the regions to which they are assigned, that will be analyzed in the continuation of the section.

To define the boundary, the first item that has to be filled out regards the **Boundary type**. In this work three boundary types are used: they are the **INFLOW** boundary, the **OUTFLOW** boundary and the **WALL** boundary. In the following, there will be analyzed first the boundaries belonging to the **WALL** type and then the other two.

**WALL BOUNDARIES**

To this category belong all the boundaries with the exception of the boundaries identified by boundary ID 1 and 2. They can be divided on the base of the surface movement type; boundaries identified by ID number 4, 5, 6 and 8, 9, 10 and 14 that make up the intake and the exhaust valve and the piston crown respectively, are moving surfaces and require a motion profile, while the others are fixed.

Intake and exhaust valves are divided in three sections (figure 4.4), i.e. stem, angle and face, to simplify temperature initialization and to allow an easier mesh local mesh refinement; this last concept will be examined in detail in section 4.2.4.

As already introduced in section 4 valves phasing and lift affect the air mass flow entering and exiting the cylinder, the in-cylinder trapped mass and thus the cylinder pressure; for this reason, these parameters have to be set carefully. The lift profile is provided as input data, and it has to be correctly phased on the base of the calibration parameters defined for this engine operating point that are reported in table 4.3.

Table 4.3 displays information related to valve phasing with two different conventions: IVO and EVC are measured with respect to the TDC firing, and being positive, they occur after it, while WNWE and WNWA are referred to the opposite TDC; also in this case they are positive, which means they occur after that TDC. From these data, it can be also seen
that the TDC firing is positioned at 0°CA as the conventionally done. Before proceeding with the valves phasing a last point has to be highlighted: opening and closing angular values are referred to a lift of 0.6 mm. This means that when the crank angle is 372.03°CA after TDC firing, the intake valve has a lift of 0.6 mm; in the same way, when the crank angle is 365.1°CA, after TDC firing, the exhaust valve has a lift of 0.6 mm. To this reference lift, a value of 0.05 mm has to be subtracted to keep in consideration the valve lash; thus, the final overall reference lift is equal to 0.55 mm and valve profiles are reported in figure 4.5.

Since the geometry surfaces are never allowed to intersect, the last task that have to be performed on the valves is the setting of the minimum lift, i.e. the lift corresponding to the closed valve; the minimum lift value suggested by the software is equal to 0.2 mm for both the intake and exhaust valves. Performed this operation, the valves geometry can be modified, as reported in section 4.2.1.

Piston motion can be either user-specified, as done with the valves or it can be directly generated by the software using the engine and the slider-crank mechanism parameters (figure 4.6).

The remainder of the WALL boundaries, and only their temperature, that will be used to model the heat transfer, has to be initialized. Table 4.4 reports the initialization temperature
For all the WALL boundaries, both the temperature and the velocity boundary conditions is of Law-of-the-Wall type. This condition is a logarithmic curve fit of a turbulent boundary layer, particularly suitable for high Reynolds number turbulent flows [44], where the viscous sub-layer is not resolved.

INFLOW AND OUTFLOW BOUNDARIES

Inflow (figure 4.7a) and outflow (figure 4.7b) boundaries constitute the actual boundaries of the system, since they define the flow going into and out of the domain.

The configurations of these two boundaries are similar, but there are some boundary conditions and options available only for INFLOW or OUTFLOW boundaries. For both of them the Dirichlet (i.e. specified value) boundary condition is set to solve the pressure equation at the boundaries, as suggested by the software manual in the case of subsonic flow; from a mathematical point of view, this condition can be expressed as

\[ \phi = f \]  

where:
Figure 4.6: Piston motion: distance of the piston crown from the BDC position

<table>
<thead>
<tr>
<th>Boundary ID</th>
<th>Boundary name</th>
<th>Temperature [K]</th>
<th>Region name</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Spark plug</td>
<td>700</td>
<td>Cylinder</td>
</tr>
<tr>
<td>4</td>
<td>Intake valve stem</td>
<td>466</td>
<td>Intake system</td>
</tr>
<tr>
<td>5</td>
<td>Intake valve angle</td>
<td>466</td>
<td>Intake system</td>
</tr>
<tr>
<td>6</td>
<td>Intake valve face</td>
<td>501</td>
<td>Cylinder</td>
</tr>
<tr>
<td>7</td>
<td>Intake port</td>
<td>369</td>
<td>Intake system</td>
</tr>
<tr>
<td>8</td>
<td>Exhaust valve stem</td>
<td>543</td>
<td>Exhaust system</td>
</tr>
<tr>
<td>9</td>
<td>Exhaust valve angle</td>
<td>543</td>
<td>Exhaust system</td>
</tr>
<tr>
<td>10</td>
<td>Exhaust valve face</td>
<td>556</td>
<td>Cylinder</td>
</tr>
<tr>
<td>11</td>
<td>Exhaust port</td>
<td>403</td>
<td>Exhaust system</td>
</tr>
<tr>
<td>12</td>
<td>Head</td>
<td>428</td>
<td>Cylinder</td>
</tr>
<tr>
<td>13</td>
<td>Liner</td>
<td>413</td>
<td>Cylinder</td>
</tr>
<tr>
<td>14</td>
<td>Piston crown</td>
<td>483</td>
<td>Cylinder</td>
</tr>
<tr>
<td>15</td>
<td>Intake valve seat high</td>
<td>369</td>
<td>Intake system</td>
</tr>
<tr>
<td>16</td>
<td>Exhaust valve seat high</td>
<td>403</td>
<td>Exhaust system</td>
</tr>
<tr>
<td>17</td>
<td>Intake valve seat low</td>
<td>369</td>
<td>Cylinder</td>
</tr>
<tr>
<td>18</td>
<td>Exhaust valve seat low</td>
<td>403</td>
<td>Cylinder</td>
</tr>
</tbody>
</table>

Table 4.4: Wall boundaries initialization temperatures

- $\phi$ is the solved quantity (e.g. pressure, velocity, temperature, species)
- $f$ is the specified value on the boundary

Here, there is the first difference between the INFLOW and the OUTFLOW boundaries; as a matter of fact, for the INFLOW boundary it is suggested to set the Neumann velocity boundary condition and specify the total pressure, from which the software calculates the corresponding static pressure. For compressible flows, the relationship between the total and static pressure is reported in formula 4.2.

$$P_{\text{static}} = P_{\text{total}} \left(1 + \frac{\gamma - 1}{2} \frac{u_i^2}{\gamma RT} \right)^{\frac{\gamma}{\gamma - 1}}$$  \hspace{1cm} (4.2)

where

- $\gamma$ is the ratio of specific heats
Figure 4.7: (a) inflow boundary (brown), (b) outflow boundary (yellow)

- $R$ is the gas constant

The Neumann boundary condition, called also specified value of the first-derivative is given by

$$\frac{\partial \phi}{\partial x} = f \quad (4.3)$$

where:

- $\phi$ is the solved quantity (e.g. pressure, velocity, temperature, species)
- $f$ is the specified derivative on the boundary

The Dirichlet boundary condition is chosen for the temperature boundary condition, too. Having specified a total pressure for the pressure boundary condition, Converge assumes that the specified temperature is the total one, and it calculates the static temperature as expressed in formula 4.4.

$$T_{\text{static}} = T_{\text{total}} \left(1, 0 + \frac{\gamma - 1}{2} \frac{u_i^2}{\gamma RT}\right)^{-1} \quad (4.4)$$

The same boundary conditions options used for the INFLOW boundary are applied to the OUTFLOW boundary, i.e. Dirichlet for pressure and temperature and Neumann for velocity boundary condition; however, in this case, the static value of both pressure and temperature are used, instead of the total ones. Figure 4.8 shows inflow and outflow pressure and temperature as a function of the crank angle; they are the same used in the validated GT-Power model.
For OUTFLOW boundaries with the Dirichlet pressure boundary condition, two ways can be adopted to dampen reflecting pressure waves in the domain:

- Specify a positive real value to assign to the parameter called predist which is then used in equation 4.5 to evaluate the static pressure at the outflow boundary through a sort of weighted interpolation of the Dirichlet pressure boundary condition $P_{\text{bound}}$ with the boundary cell pressure $P_{\text{fluid}}$

$$P_{\text{static}} = \frac{P_{\text{bound}} + \text{predist} \cdot P_{\text{fluid}}}{1 + \text{predist}}$$  \hspace{1cm} (4.5)

- Specify a sponge layer based on the formulation of Bodony [45]

The software guide suggests to adopt one of these two methods only if results are affected by unrealistic pressure waves; for this reason, they were not taken into account from the beginning, but they will be introduced if needed.

For what concerns the species boundary condition, to faithfully replicate the experimental conditions, differently from what done in the spray calibration section, air pulled into the domain, is not completely dry, but it has a small amount of water vapour as reported in table 4.5.
<table>
<thead>
<tr>
<th>Species name</th>
<th>Mass fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>$O_2$</td>
<td>23.14%</td>
</tr>
<tr>
<td>$N_2$</td>
<td>76.17%</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>0.69%</td>
</tr>
</tbody>
</table>

Table 4.5: Inflow boundary condition species and respective mass fractions

Finally, for both INFLOW and OUTFLOW boundaries, the initialization values of the turbulent kinetic energy $k$ and of the turbulent dissipation $\varepsilon$ have to be defined. The turbulent kinetic energy can be evaluated as

$$k = \frac{3}{2} u_i^2 I^2$$  \hspace{1cm} (4.6)

where

- $I$ is the turbulence intensity, typically in between 0.05 and 0.20 for engines
- $u_i$ is the local velocity

and the turbulent dissipation rate $\varepsilon$ can be evaluated as

$$\varepsilon = \frac{c_{\mu}^{3/4} k^{3/2}}{\text{lengthscale}}$$  \hspace{1cm} (4.7)

where

- $c_\mu$ is a modelling constant equal to 0.09
- the lengthscale can be approximated by the 10% of the hydraulic diameter

Since there's no guarantee that $k$ and $\varepsilon$ values obtained through formula 4.6 and 4.7 are sufficiently precise, the strategy adopted here, is to maintain the values suggested by the software, i.e. $k = 0.02$ and $\varepsilon$ evaluated by the software starting from a value of the lengthscale equal to 0.003 m, setting the start time of the simulation with a certain advance, so that these initialization values have enough time to converge to their actual value.

After having modified the geometry and defined all the boundaries, it is possible to correctly define the BDC and TDC piston position through the compression ratio calculator tool; as a matter of fact, the minor geometry modifications can lead to the variation of the TDC cylinder volume, but the software, knowing the target compression ratio and the kinematics of the crank mechanism, slightly translates the piston in order to counterbalance these changes.

At this point, the boundaries can be assigned to the regions: as anticipated, the main goals of the regions are to allow an easy variables initialization and to set events, such as the opening and closing of intake and exhaust valves. In the light of this last statement, the regions defined are three, i.e. Intake system, Exhaust system and Cylinder, and the boundaries that belong to each of them are reported in tables 4.2 and 4.4 and highlighted in figure 4.9 with three different colors.

Two cyclic events are defined to simulate the intake and exhaust valves opening and closing. The intake valves motion has to do with the Cylinder and the Intake system regions, while the exhaust valves motion with the Cylinder and the Exhaust system. From the lift
profiles defined, the software automatically fills out the start and the end of the processes, which coincide with the removal and the creation of the disconnected triangles. Table 4.6 contains the value of the regions initialization variables, whose temperature and pressure values are equal to the ones of the \textit{INFLOW}, \textit{OUTFLOW} and \textit{WALL cylinder} boundaries respectively. As already said for \( k \) and \( \varepsilon \), it’s is not fundamental that they are extremely accurate, since the first 180 °CA of the simulation are, by design, allocated for the variable stabilization process.

<table>
<thead>
<tr>
<th>Region</th>
<th>Temperature [K]</th>
<th>Pressure [bar]</th>
<th>TKE ([m^2/s^2])</th>
<th>(\varepsilon) [m^2/s^3]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cylinder</td>
<td>1457.3</td>
<td>9.36</td>
<td>1.0</td>
<td>100.0</td>
</tr>
<tr>
<td>Intake system</td>
<td>323.1</td>
<td>2.20</td>
<td>1.0</td>
<td>100.0</td>
</tr>
<tr>
<td>Exhaust system</td>
<td>1521.8</td>
<td>5.09</td>
<td>1.0</td>
<td>100.0</td>
</tr>
</tbody>
</table>

Table 4.6: Regions initialization values

4.2.3 Spray rate and orientation

In section 3.6 are reported the injection model parameters that are used for the engine simulation. What has to be defined now, is the injection profile for an injection pressure of 200 bar. The procedure is the same used to evaluate the mass flow rate for an injection pressure of 160 bar (equation 3.8); the mass flow rate provided at 100 bar is scaled by the square root of the pressure ratio as reported in formula 4.8.

\[
q_{200\text{bar}} = q_{100\text{bar}} \sqrt{\frac{200}{100}}
\]  

(4.8)

The end of the injection is established so that the cumulative injected mass is equal to the target one, whose value is computed starting from the fuel mass flow rate measured on the test bench for this specific engine working point (formula 4.9).

\[
m_{\text{inj}} = \frac{q_{\text{fuel}} \cdot m}{\omega \cdot i} = \frac{0.0492 \cdot 2}{116.67 \cdot 8} = 1.06 \cdot 10^{-4} \text{kg}
\]  

(4.9)

where
- $q_{fuel}$ is the measured fuel mass flow expressed in kg/s
- $m$ is the number of crank revolutions for each power stroke, equal to 2 for 4-stroke engines
- $\omega$ is the engine speed expressed in rsp
- $i$ is the number of cylinders, equal to 8

With the results obtained through formulas 4.8 and 4.9, the injection period is computed; the injection profile is plotted as a function of injection in figure 4.10.

![Figure 4.10: Injection rate for an injection pressure of 200 bar as a function of the injection time](image)

The start of injection occurs 360 °CA before TDC firing, and the fuel injected is the CONVERGE standard gasoline, Gasoline_CSI.v1. The origins of the injector are equally spaced on a circumference of radius 0.5 mm lying on a plane 0.5 mm far from the injector cavity. The $z$ (figure 3.2) axis of the injector is 26° tilted with respect the squish plane with beams 1 and 7 (figure 3.2) pointing higher that beams 3 and 5. This configuration is defined according to the objective of avoiding spray intersections with the intake valves, when these are at their maximum lift (about 10 mm).

### 4.2.4 Grid control

With respect to the grid used for the spray calibration, here the base grid dimension is set equal to 2 mm instead of 16 mm. This choice mainly derives by the fact that the computational volume is smaller and that the phenomena to be studied is not limited to a portion of the volume. With this base grid settings, the software forecasts 82520 cells. Then the following fixed embeddings volume are applied:

- **CYLINDER:** permanent cylindrical volume centered with the cylinder axis, with a radius of 50 mm and an height of 150 mm, so that it embeds all the cylinder, even with the piston at the BDC, and a sector of the intake and exhaust systems. The embedding scale is equal to 1, which means that the grid is made up of 1 mm$^3$ cells.

- **INJECTOR:** cyclic embedding with embedding scale equal to 2 (cells of 0.5 mm side), focused on the injector beams. Their function is to replicate the same minimum grid size used in the spray calibration procedure.
Figure 4.11: Injection orientation: (a) frontal view, (b) lateral view, (c) view perpendicular to the injector z axis (26° titled with respect the horizontal plane)

- **INTAKE and EXHAUST VALVES ANGLES AND SEATS**: these two embeddings are applied to their relative boundaries, i.e. the ones identified by ID numbers 5, 9, 15 and 16 in table 4.4; they have embedding level equal to 3 (cells of 0.25 mm side). They are activated to better support the process of creation and removal of the disconnected triangles and to capture possible edge effects.

- **SPARK PLUG**: two spherical embeddings with embedding level equal to 3 with activation time that goes from 700 to 720 crank angles, but different radius, 2 and 4 millimeters respectively.

Figure 4.12: Engine simulation embeddings: (a) frontal view, (b) lateral view

For what concerns the AMR, it is applied in the three regions, with different application
settings and maximum number of cells in the computational volume equal to 7 millions:

- **CYLINDER**: permanent AMR with the same criteria used for the spray calibration; maximum embedding level equal to 3; cells can have a side of 0.25 mm at most.

- **INTAKE AND EXHAUST SYSTEM**: cyclic AMR that activate with the intake and exhaust phase respectively. The only variable field that determines its activation or deactivation is the velocity, since it’s goal is to better reproduce air motion in the intake and exhaust ports. The embedding level is equal to the one used for the cylinder.

### 4.2.5 Summary

Figure 4.13 reports the main important events, as set in the model, to be studied in this preliminary simulation.

![Figure 4.13: Intake and exhaust valves lift and injection profile as a function of the crank angle](image)

With reference to figure 4.13, the intake valves open at 357.95 °CA and closes at 612.78 °CA, while the exhaust valves open at 136.77 and closes 391.61 °CA. Injection starts 360 °CA before TDC firing and lasts 201.81 °CA, i.e. until 561.81 °CA.

A .map file, i.e. the file containing all the simulation variables in a specific instant, is written for a crank angle equal to 357 °CA; this file is usually written few crank angles before the air-fuel charge is ignited; in this case, instead it is written few crank angles before the SOI since in the complete cycle simulation different hydrocarbons blends will be tested in order to replicate the experimental results.
4.3 Cold cycle results

4.3.1 Cylinder trapped mass

The first goal of the cold cycle simulation is to check the correct phasing between the valves phasing and the imposed boundary conditions, since their relation influences the air flow and thus the in-cylinder trapped mass. In Converge, all the output related to region-to-region mass flow are reported into the file `region_flows.out`. As said, simulation starts with the exhaust valve partially opened; this causes the mass flow from the cylinder to the exhaust system to oscillate until the turbulent kinetic energy, the turbulent dissipation and the turbulent fluctuations, that influence the velocity field, stabilize.

![Figure 4.14: Cold cycle exhaust mass flow and exhaust valves lift profile as a function of crank angle](image)

The value of the mass flow is positive when the the charge moves from the cylinder to the exhaust port; it can be seen that almost 90 °CA are required to have the CFD results converging to the experimental ones. After the expansion phase, when the exhaust valves open again, the mass flow assumes negative values, which means that the mass is moving from the exhaust port toward the cylinder; this is due to the fact that, the cylinder pressure remains below the expected one, since combustion is omitted.

The same analysis can be performed on the intake mass flow, whose results are reported in figure 4.15.

![Figure 4.15: Cold cycle intake mass flow and intake valves lift profile as a function of the crank angle](image)
It can be seen that the CFD mass flow is slightly delayed with respect to the experimental one; after this initial phase, the computed mass flow becomes larger of a small amount, keeping however a good match with the experimental values especially for what concerns the trend and the peak value. During the closing phase of the intake valve, the two lines almost coincide, leading to an overall good match.

As said in section 4.2.2, valves open and close when the value set in the valve motion file is equal to the minimum lift value; this event is highlighted by the two sharp steps present near to the opening and closing phases (figure 4.16).

Figure 4.16: Cold cycle intake mass flow rate, focus on the opening and closing phases

The correctness of the simulated gas exchange processes allows to get extremely good results related to the cylinder trapped mass (figure 4.17). At the beginning of the simulation, the error with respect the experimental results is not negligible. However, as it happens for the exhaust mass flow, after some crank angles, the simulation results converge to the experimental ones. At the TDC firing, the simulation amount of trapped air is equal to 1,3596 g, while the experimental value is of 1,3528 g, leading to a relative error of 0,5%.

Figure 4.17: Cold cycle trapped mass as a function of the crank angle

4.3.2 Cylinder thermodynamic conditions

Mainly two conditions are required to replicate the experimental pressure trace on a cold cycle simulation; these are the correct definition of the compression ratio and of the cylinder trapped mass (section 4.3.1). Furthermore, heat transfer and thus in-cylinder temperature,
can contribute to this goal. Figure 4.18 shows the cold cycle cylinder pressure; it's compared to the experimental pressure trace obtained in the firing cycle. Thus, the comparison has to be performed on the cycle until the start of combustion; at this timing, the difference is smaller than 1 bar, a result that can be considered acceptable.

Figure 4.18: Cold cycle cylinder pressure as a function of the crank angle

A general overview of the cylinder thermodynamic data is provided by the logarithmic Clapeyron diagram, reported in figure 4.19. The simulation starts at the beginning of the exhaust stroke (A) and a small discrepancy with the experimental data is obtained when the piston reaches the TDC at the end of the exhaust stroke (B). However, as already shown in figure 4.17, at the end of the intake stroke (C), the amount of trapped mass is correct, and during compression, the simulation curve faithfully follows the experimental one. At the end of the compression stroke (D), the simulated curve traces again the path followed during compression, because in the cold cycle simulation, the system behaves as an air spring. Actually the curve during the expansion stroke, from (D) to (E), doesn’t coincide with the curve obtained during the compression stroke, but it’s slightly below it, since the simulation keeps into account also the heat exchanges, making the process not perfectly adiabatic.

Figure 4.19: Cold cycle logarithmic Clapeyron diagram
To assess the heat exchange processes between the charge and the surface walls, as done with the pressure, also cylinder temperatures can be compared, as reported in figure 4.20. With respect the GT data, there is a large inconsistency about 360 °CA before TDC firing due to the different nature of the calculation, but as the compression stroke proceeds, this difference is reduced, and at the spark discharge event, the difference is smaller than 20 K.

Figure 4.20: Cold cycle cylinder temperature as a function of the crank angle

Results shown up to now doesn’t provide a detailed view of all the in-cylinder processes; they are rather used to verify if some macroscopical deviations from the experimental values are present. Moreover, these aspects are common to many kinds of engine; thus, in sections 4.3.3 and 4.3.4 a more detailed analysis on the most peculiar parameters of GDI engines is reported.
4.3.3 In-cylinder motion

GDI engines are usually tumble-based, i.e. designed to obtain an organized charge motion about an axis perpendicular to the cylinder axis. Tumble is obtained during the intake phase, through a suitable design of the intake ports; usually as the piston reaches the BDC, the tumble intensity decreases, but then, it is enhanced again during the compression stroke; finally it is converted into turbulent kinetic energy before the start of combustion helping in getting a faster combustion process.

Tumble about the $y$ axis (parallel to the crankshaft) is called normal tumble, while tumble about the $x$ axis is called cross tumble. Figure 4.21 shows the axes with respect normal and cross tumble and swirl are computed; the positive and negative rotation directions are defined according to the right hand rule.

Figure 4.21: Rotation axes used for defining normal (blue) and cross tumble (red) and swirl (green)

The tumble intensity is defined through the tumble ratio, evaluated as the ratio between the angular speed of the flow about the center of mass and the crankshaft angular speed as shown in equation 4.10, referred to the normal tumble.

$$\text{tumble ratio} = \frac{\omega_y}{\omega_{crankshaft}} \quad (4.10)$$

As in most GDI engines, the swirl is negligible during the whole cycle, whereas tumble is predominant. The overall cross tumble is almost equal to zero, due to symmetry reasons of the intake port. Thus, the normal tumble is the predominant charge organized motion.
In figure 4.22, the initial oscillations, from 180 to 270 CA are related to the oscillations in the exhaust flow rate due to the stabilization of the field variables (figure 4.14). As the intake valve opens, a positive (same direction of rotation of the crankshaft) tumble of reduced intensity is generated; this is due to the deflection toward the injector of the flow entering the combustion chamber (figure 4.23a). In the same period, the turbulent velocity and thus the turbulent kinetic energy, steadily increase as the result of the piston acceleration toward the BDC; the fast increase of turbulent velocity is also magnified by the interaction between the in-cylinder air and the spray injected at high pressure [46]. As the intake valves lift increases (figures 4.23b and 4.23c), the majority of the flow is deflected toward the opposite side of the cylinder, i.e. toward the exhaust valves, resulting in a tumble sign changeover, from positive to negative. The gradual closure of the intake valves leads to a reduction of the tumble intensity, that however slightly increases during the compression stroke from 135 °CA to 70 °CA before the TDC firing (figures 4.23d and 4.23e). In this angular interval, a different trend in the turbulence intensity can be observed; as a matter of fact, turbulences generated during the first phases of the intake valves opening steadily decreases from 250 °CA to 90 °CA before TDC firing; from this point on, the destruction of the tumble results in a temporary stabilization of the turbulence level.
Figure 4.23: Cylinder flow field on the plane passing through the intake valve axis: 410 °CA (a), 450 °CA (b), 530 °CA (c), 640 °CA (d) and 410 °CA (e).
An important parameter affecting engine performances is the turbulent kinetic energy close to the spark plug: the increase of the TKE near to the spark plug increases the combustion starting velocity, reducing combustion duration and thus improving efficiency [47]. The increase of the TKE and thus of the turbulent velocity fluctuations near the spark plug has the effect of moving the operating point on the Borghi plot toward the upper boundary of the thin reacting zone; this results in the increase of the turbulent flame speed under the same operating conditions (e.g., equivalence ratio, thermodynamic conditions and thus laminar burning speed). In figure 4.24 is shown the turbulent kinetic energy evaluated in a cubic volume with the same volume of a sphere with a radius of 4 mm, compared to the volume averaged in the entire cylinder.

![Figure 4.24: Comparison of the turbulent kinetic energy averaged over the cylinder and over the monitor point](image)

In figure 4.25, the turbulent kinetic energy is plotted on two orthogonal planes that coincide with the tumble plane passing through the cylinder axis and the swirl plane passing through the spark plug gap. It can be seen that near the walls, where velocity fluctuations are dampened by the viscous interaction between the in-cylinder charge and the geometrical surface, the turbulent kinetic energy reaches its minimum value, while higher values are obtained closer to the spark plug. Two symmetrical local maxima can be highlighted in the vicinity of the xz planes coincident with the intake valves axis as result of the conversion process of the energy conveyed by the tumble in turbulent fluctuations. The influence of the turbulent velocity fluctuations and of the motion pattern of the in-cylinder charge on the flame front propagation are reported in section 5.3.
4.3.4 Spraying orientation and distribution

Since the injection occurs during the intake phase, when the intake valves are open, the combustion chamber is designed to reduce as much as possible spray-valves interaction. This results in some advantages, such as the reduction of the mixture temperature and a more precise control of the actual in cylinder air to fuel ratio (AFR). A qualitative analysis can be performed looking at the spray morphology during injection, focusing on the cycle crank angles corresponding to the maximum intake valves lift. As shown in figure 4.26, at 480 °CA, the intake valves have reached their maximum lift and the injected fuel doesn’t target directly the valves.

The output file film_accum.out lists the amount of fuel that has made contact with a boundary, while the output file film_accum_net.out gives the parcel mass that has reached a boundary and remained on it. In particular, for what concerns the intake valve angle and the intake valve face boundaries, results are reported in figure 4.27.
At the end of the injection, the total amount of fuel that has interacted with the intake valves angle and face is equal to $6.46 \times 10^{-7}$ kg, and the amount of fuel remained on these two boundaries is equal to $2.21 \times 10^{-7}$ kg. These quantities represent the 0.61% and the 0.21% respectively of the total amount of fuel injected, equal to $1.06 \times 10^{-4}$ kg. Moreover, it can be seen that, the interaction between the liquid fuel and the intake valve angle occurs after the end of the injection, as result of the in cylinder charge motion.

In air-guided GDI engines, the interaction between spray and fresh air helps the fuel-air mixing process. During the first phases of the injection (figure 4.28a), the injected fuel impinges on the piston crown; part of it slides on the piston and the other part is reflected toward the center of the combustion chamber according to the tumble direction. This trend continues until the tumble motion is positive, i.e. generated by the flow entering the cylinder from the liner side (figure 4.28b). As the piston moves toward the BDC, the tumble reverses its rotational direction and two main vortices are generated (figure 4.28c); finally, these two vortices merge in a single vortex that influences the spray distribution even after the end of the injection (figure 4.28d).

From the above description of the spray morphological evolution, related to the in-cylinder motion, it can be seen that during the first phases of the injection, the spray is partially deflected toward the intake port by the initial positive tumble; this makes that, at the end of the intake phase, $1.80 \times 10^{-6}$ kg of fuel, that corresponds to 1.69% of the total amount of fuel injected, has moved into the intake ports.

Spray interaction with liner and piston crown plays a fundamental role in the mixture formation process; as a matter of fact fuel deposits increase particulate matter and unburned hydrocarbon emissions and the liquid impacting on the liner results in an increased oil dilution. In figure 4.29 it can be seen that, as the injection starts with the piston at TDC (360 °CA before TDC), a large amount of liquid mass hits the piston crown; however, most of this fuel fraction doesn’t remain on the piston surface, but rebounds according to the Wall film model. As the piston moves toward the BDC, the mass of fuel that interacts with it reduces, but then increases again as the piston approaches the TDC. In this last phase, the curve showing the net cumulative mass doesn’t increase as you might expect: this is probably due to the fact that during compression the temperature increases above the Leidenfrost temperature, i.e. the temperature at which vapour production prevents wall wetting (figure 4.28a).

Regarding the liner, the first liquid droplets interact with it about 90 °CA after the start of injection. Then the liquid film mass increases for about 40 °CA after the end of injection, and then fastly decreases as the piston approaches the TDC (figure 4.28b).
Finally, spray distribution affects the local equivalence ratio in the combustion chamber; mixture inhomogeneities can lead to over-lean or over-reach zones, resulting in potential combustion-related issues (e.g., bulk quenching) and an increase of pollutants formation. This aspect is analyzed in section 5.3, and referred to the surrogates that provides the best...
results in term of pressure trace and heat release rate.
Chapter 5

Combustion simulation

In spark ignition engines combustion starts near the spark plug thanks to the spark discharge event and results in the generation of a partially ionized plasma channel at high temperature [48]. The expansion of the flame kernel continues thanks to the heat conduction occurring from the high temperature burned gas region (2000-2500 K) toward the unburned region. The area in which this phenomena occur is called flame front and can be divided in three regions:

- Preheat zone
- Inner layer
- Oxidation layer

In the preheat zone the temperature increase, obtained through heat conduction from the burned region, promotes the partial oxidation of the fuel with the oxygen. From these low temperature reactions, active radicals, responsible for the chain branching reactions occurring in the inner layer, are produced; in the oxidation layer, the products of the previous reactions are oxidized through chain breaking reactions.

In absence of turbulent motions, the propagation of the flame front would be rather slow (some tens of centimeters per second) and thus unsuitable for internal combustion engine applications. Correlations between the relative air to fuel ratio, pressure and temperature and the laminar burning speed in a spherical closed vessel are provided by [49]. However, in internal combustion engines, combustion is not laminar, but it is turbulent; thus, the flame front is distorted by both relatively large and small scales wrinkles. Turbulences increase the scalar mixing and thus the flame front propagation speed increases up to 20-40 m/s on the base of the operating condition.

5.1 Combustion model

The validation of the cold-cycle simulation is just the starting point towards the engine cycle simulations; as already discussed in chapter 4, any particular tuning of the model parameters was performed, but the attention was mainly focused on the correctness and congruence (e.g. correct phasing between valves lift profiles and boundary conditions) of the many model input parameters.

At this stage of the work, the two main issues to be addressed are the definition of the fuel,
and the choice of the combustion model. Among the different models available in literature, such as the G-equation, the ECFM, etc., the choice fell on the SAGE Detailed Chemical Kinetics solver. The reasons for choosing the SAGE model are the following:

- It doesn’t require any particular tuning; the only adjustable parameters are the Prandtl and the Schmidt numbers, which influence the species diffusion phenomena. Moreover, a calibration procedure performed on a single working point could lead to unreliable results.
- It can be employed for the simulation of abnormal combustion processes.
- There exist many reaction mechanisms with extremely good agreement with the experimental tests able of replicating the combustion of gasoline surrogates.

The biggest disadvantage is the increase of the computational time with respect to the other mentioned models.

### 5.1.1 SAGE Detailed Chemical Kinetics solver

Any chemical reaction can be described as a series of elementary reactions that can be written as [50]

\[
\sum_{j=1}^{J} v'_{ji} \chi_j \Leftrightarrow \sum_{j=1}^{J} v''_{ji} \chi_j \quad \text{for} \quad i = 1, 2, \ldots, I
\]  

(5.1)

where:

- \(v'_{ji}\) and \(v''_{ji}\) are respectively the reactants are products stoichiometric coefficients for species \(j\) and reaction \(i\)
- \(\chi_j\) is the chemical symbol for the species \(j\)
- \(I\) is the total number of reactions

The net production rate of the \(j\)-th species \(\dot{\omega}_j\) is given by

\[
\dot{\omega}_j = \sum_{i=1}^{I} v_{ji} q_i \quad \text{for} \quad j = 1, 2, \ldots, J
\]  

(5.2)

where

- \(v_{ij} = v''_{ji} - v'_{ji}\)

(5.3)

- \(q_i\) is the rate-of-progress parameter for the \(i\)-th reaction and is defined as a function of the species molar concentration \([X_j]\) and of the forward \(k_{fi}\) and reverse \(k_{ri}\) rate coefficients for reaction \(i\), as reported in formula 5.4

\[
q_i = k_{fi} \prod_{j=1}^{J} [X_j]^{v'_{ji}} - k_{ri} \prod_{j=1}^{J} [X_j]^{v''_{ji}}
\]  

(5.4)
The forward rate coefficient is expressed through the Arrhenius form

$$k_{fi} = A_i T^{b_i} \cdot \exp\left(-\frac{E_i}{R_u T}\right)$$  \hspace{1cm} (5.5)$$

where

- $A_i$ is the pre-exponential factor
- $b_i$ is the temperature exponent
- $E_i$ is the activation energy
- $R_u$ is the universal gas constant

The reverse rate coefficient, reported in formula 5.6 can be calculated from the equilibrium coefficient $K_{ci}$ determined on the base of thermodynamic properties.

$$k_{ri} = \frac{k_{fi}}{K_{ci}}$$  \hspace{1cm} (5.6)$$

Knowing the above relations, the mass (equation 5.7) and the energy (equation 5.8) conservation equations can be solved for each cell of the computational domain.

$$\frac{d[X_j]}{dt} = \dot{\omega}_j$$  \hspace{1cm} (5.7)$$

$$\frac{dT}{dt} = \frac{V \frac{dp}{dt} - \sum_j (h_j \dot{\omega}_j)}{\sum_j ([X_j] c_{p,j})}$$  \hspace{1cm} (5.8)$$

where

- $h_j$ is the molar specific enthalpy of the $j$-th species
- $c_{p,j}$ is the molar constant-pressure specific heat of the $j$-th species

The last part of this section is devoted to the description of the kinetic mechanism used in this work, and it’s prediction capabilities of simulating combustions of toluene reference fuels (TRF), acting as a link with the topic covered in section 5.1.2.

In literature can be found many mechanisms able to reproduce gasoline combustion processes; in [51] different kinetic mechanisms are tested and compared to experimental shock tube ignition delays. The kinetic models under study are the Mehl et al. mechanism, the Wang et al. mechanism, the Cai et al. mechanism and the Andrae mechanism; among these, the Andrae mechanism shows the lowest mean absolute ignition delay relative error, of about 20.05%, and for this reason it is chosen also in this work to manage combustion processes.

It is made up of 159 species and 734 reactions. The original version of the mechanism was updated in [52] to revise and improve chemical kinetic models for toluene reference fuels and then in [53] to evaluate the impact of adding an olefin to a TRF.

The high accuracy of the model, summed to its capability of replicating gasoline surrogates with different properties in different operating conditions, directed the mechanism choice toward the Andrae 2016 kinetic mechanism.
5.1.2 Toluene reference fuel

The definition of the composition of the injected fuel affects the blend properties and thus the combustion mechanism. Gasoline is made up of hundreds of compounds (mixture of n-paraffins, i-paraffins, cyclo-paraffins, olefins and aromatics), for which a complete detailed chemical description is unfeasible; thus, the actual compound is defined through a restricted set of compounds able to emulate the behaviour and characteristics of the actual fuels.

Up to now, the Converge standard gasoline CSI\textsubscript{Gasoline, v1}, whose composition and properties are defined in table 3.5 and in figure 3.7, was used to carry on simulations, and iso-octane was defined as the only vapour species of this gasoline surrogates. Properties of CSI\textsubscript{Gasoline, v1} and i-octane, shown in figure 3.7, are rather similar, but they show some not negligible differences too (e.g. density); moreover, they don’t provide a complete picture of the blend, especially for what concerns combustion characteristics. For this reasons, the blend has been changed and different attempts are performed with different surrogates in order to find the one that better match with the experimental conditions. Here, the focus of the study is shifted toward that properties that directly affect combustion processes, such as the octane number (ON), the lower heating value (LHV), the stoichiometric air to fuel ratio $\alpha_{st}$ and finally the density $\rho$.

Regarding these, the target to be achieved, experimentally determined are reported in table 5.1.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>98</td>
</tr>
<tr>
<td>LHV</td>
<td>42.63 [MJ/kg]</td>
</tr>
<tr>
<td>$\alpha_{st}$</td>
<td>14.17</td>
</tr>
<tr>
<td>$\rho$</td>
<td>727 [kg/m$^3$]</td>
</tr>
</tbody>
</table>

Table 5.1: Ferrari surrogate gasoline properties

Usually, in spark ignition engines primary reference fuels of n-heptane and i-octane are used as surrogates [54], since they are able to correctly describe autoignition and heat release. To keep into account of the gasoline aromatic compounds, toluene is added to n-heptane and iso-octane, resulting in a ternary reference fuel [55], [56]. In [57] laminar burning velocity of a commercial gasoline is measured over different thermodynamic and operating conditions and compared to the laminar burning velocity of two gasoline surrogates, a primary reference fuel (PRF) and a TRF; over the entire range of operating conditions the TRF shows better agreement with the experimental results. In the present work, different TRF surrogates are tested in order to replicate the experimental results.

The octane number is an indicator of the knocking propensity of a specific compound; it indicates the amount, on a volume percentage basis, of i-octane in a blend of i-octane and n-heptane which shows the same knock intensity of the fuel under investigation. Two different types of octane number can be defined:

- **Research ON (RON)** is evaluated in a test engine running at 600 rpm, intaking air at 53 °C, with a spark advance of 13 °CA (ASTM D2699); it is representative of city driving conditions
- **Motored ON (MON)** is evaluated in a test engine running at 900 rpm, intaking air at 149 °C, with a spark advance in between 26 and 14 °CA as a function of the cylinder height (ASTM D2700); it is representative of highway driving conditions
Usually, standard gasolines have an higher RON than its corresponding MON, and their difference is called fuel sensitivity, denoted by the letter S.

\[ S = RON - MON \] (5.9)

In the following paragraphs a short description of two methodologies by Morgan et al. [31] and by Ghosh et al. [58] used in the present work to define RON and MON of a specific TRF is reported.

MORGAN ET AL. METHODOLOGY

This methodology can be divided in three phases; the first phase consists in the experimental determination of the octane number through the conventional procedure: the fuel is tested and compared to two reference fuels, one with an ON slightly higher and the other one with an ON slightly lower. Then the octane number of the fuel is determined by linear interpolation using formula 5.10

\[ ON_{test} = ON_{PRF-L} + \left( \frac{KI_{PRF-L} - KI_{test}}{KI_{PRF-L} - KI_{PRF-H}} \right) + (ON_{PRF-H} - ON_{PRF-L}) \] (5.10)

where

- \( KI_{PRF-L} \) is the knock intensity of the PRF that gives an ON slightly lower than the tested fuel
- \( KI_{PRF-H} \) is the knock intensity of the PRF that gives an ON slightly higher than the tested fuel
- \( KI_{test} \) is the knock intensity of the tested fuel
- \( ON_{PRF-L} \) is the octane number of the PRF that gives an ON slightly lower than the tested fuel
- \( ON_{PRF-H} \) is the octane number of the PRF that gives an ON slightly higher than the tested fuel

The second step consists in the definition of fitting response surfaces, i.e. surfaces for which, given a TRF composition, a unique ON can be defined; three different models are presented:

- Linear-by-volume model
- Second order model
- Modified linear-by-volume model

The study shows that, among the three models, the linear-by-volume model is the one that introduces the largest error; the second order model provides almost the same results of the modified linear-by-volume model with larger complexity and an higher number of free parameters. This led the authors to use the modified linear-by-volume model, whose mathematical formulation is reported in formula 5.11.

\[ RON = a_p + a_{tol}v_{tol} + a_{tol}v_{tol}^2 + a_{tol,p}v_{tol}p \] (5.11)

where
\[ p = \frac{v_i}{v_i + v_{nH}} \]

\[ v_i \text{ is the volume fraction of the } i\text{-th component} \]

The third step is the reverse procedure of what done up to now; as a matter of fact it is provided a methodology to define the fuel composition to emulate a specific RON and MON.

Of particular interest for this work is the fuel surrogate with an experimentally evaluated RON of 98.5 and MON of 88.0, whose composition is: 5.833 vol % of i-Octane, 18.749 vol % of n-Heptane and 75.418 vol % of Toluene.

**GHOSH ET AL. METHODOLOGY**

The choice of this methodology came from the flexibility and accuracy of the model; as a matter of fact, it is able to predict the octane number, over a wide octane range (from 30 to 120), within a standard error of 1 number for both RON and MON, independently on the refining process stream used to obtain the specific gasoline. The most important concepts and mathematical steps on which this methodology is based on, are given in this section, whereas a complete description is reported in [58].

Each gasoline is made up of many different hydrocarbon molecules; each of them contributes to the mixture ON on the base of its blend value \( B_{ON}^i \).

\[ ON = \sum_i v_i B_{ON}^i \]  

where \( v_i \) is the volume fraction of the \( i \)-th component in the blend. Experimental studies show that the blend value of a specific component is proportional to the ON of the gasoline to which it belongs; thus, on the base of this, equation 5.13 can be written

\[ B_{ON}^i = a_{i}^{(0)} + a_{i}^{(1)} (ON) \]  

One of the two parameters of equation 5.13, \( a_{i}^{(0)} \) and \( a_{i}^{(1)} \), can be eliminated exploiting the special case in which the gasoline fuel is a pure-component fuel; in this case, the fuel has the same ON of the pure-component, that coincides with the blend value too. Through the application of this constraint, equation 5.13 can be rewritten as

\[ ON_i = a_{i}^{(0)} + a_{i}^{(1)} (ON_i) \rightarrow a_{i}^{(0)} = (1 - a_{i}^{(1)}) ON_i \]  

Defined \( \beta_i = 1 - a_{i}^{(1)} \), equation 5.14 becomes

\[ a_{i}^{(0)} = \beta_i ON_i \]  

Finally, combining equations 5.12, 5.13 and 5.15, the basic octane prediction model is obtained.

\[ ON = \sum_i v_i \beta_i ON_i \sum_i v_i \beta_i \]  

This formulation can be applied to obtain ON of mixture made up of a single molecular class (e.g. paraffins, olefins, naphthenes, aromatics). However, when dealing with blends made up of different molecular classes, the interaction among the components can be non-linear (figure 5.1).
Figure 5.1: positive interaction (a), no interaction (b) and negative interaction (c) between two species

To keep in to account this deviance, a function on purpose can be defined; for a binary mixture, it takes the formulation reported in equation 5.17.

\[ y = \frac{k_{12}^a v_1 v_2}{1 + k_{12}^b v_2} \]  

(5.17)

where \( k_{12}^a \) and \( k_{12}^b \) are the interaction parameters. Due to the fact that the number of interaction parameters increases extremely rapid with the number of lumps used to represent the gasoline, only interaction between paraffins and naphtenes and between paraffins and olefins are considered. With the same procedure followed in the first phase of this section, equation 5.18 is obtained.

\[
ON = \frac{\sum_{PONA} v_i \beta_i ON_i + I_P \sum_P v_i \beta_i ON_i}{\sum_{PONA} v_i \beta_i + I_P (\sum_P v_i \beta_i - \sum_P v_i)}
\]

(5.18)

where \( I_P \) is the interaction term defined as

\[
\left( \frac{k_{PN}^{(a)} v_N + k_{PO}^{(a)} v_O}{1 + k_{PN}^{(b)} v_N + k_{PO}^{(b)} v_O} \right)
\]

(5.19)

The estimation of the parameters of 5.18 was performed over a set of 1471 gasolines obtained from different refining processes through a constrained least-squares minimization procedure.

5.2 Combustion simulation setup

Most of the model inputs have been already implemented during the cold cycle simulation; what is still missing are the spark event definition and the combustion model implementation. To the first one is addressed the task of simulating the ignition of the mixture, whereas to the latter the simulation of the combustion process.

5.2.1 Source modelling

In spark-ignition engines, combustion doesn’t start spontaneously, but it is started by an electrical breakdown discharge. In literature can be found many studies on the influence that the spark energy and power and the geometrical features of the electrode, such as width,
shape and gap size have on the development of the flame kernel (e.g. [59], [60]). Being this work focused on the entire engine simulation, rather than on this particular aspect, whose overall influence on the numerical simulation is limited, the best practices suggested by the software are employed.

In *Converge*, the sparking is simulated through the imposition of an energy source. From a macroscopic point of view the spark event can be seen as a single process; however, if observed from a microscopic point of view, it’s the result of many subprocesses, that can belong to the high current phase and to the low current phase. At the beginning of the process, the voltage ramps up across the spark gap; when the breakdown voltage is reached, a surge of power is released and the voltage suddenly drops down. The remaining energy is released during the arc and glow phase.

![Figure 5.2: Example of a voltage curve during a spark event, [61]](image)

The behaviour of the voltage across the spark splug can be modelled through an equivalent electrical circuit made up of resistances and capacitances; being the number of parameters to be tuned large and dependent on composition, dimensions and geometrical features of the injector unknown, a simpler model is employed. The complex curve reported in figure 5.2, from which derives the energy released by the spark can be simplified dividing it into two regions; the first region models the high power phase and the second one the low power phase.

For this purpose, two energy sources providing the same energy amount, equal to 20 mJ, but different durations (0.5 °CA for the high power phase and 10 °CA for the low power phase) are employed and applied on a spherical volume of 0.45 mm centered with the spark axis (figure 5.3).

Two ignition time are tested, one coincident with the command of the control unit and the second one retarded of 0.75 CA degrees that keeps into account of the retard between electronic control unit (ECU) signal and command actuation (e.g. anti-knock control).
5.2.2 Combustion setup

In section 5.1.1 the theoretical background of the model is shown, while in this section, the setting used in this work is reported. To expedite the computations, a cutoff temperature equal to 600 K and a minimum mole fraction of CO, $H_2$ and hydrocarbon species equal to $1e-10$ are imposed. In the computational cells with lower temperature and HC species mole fraction of the ones reported, the detailed chemistry calculator doesn’t work. The name of the fuel species is defined according to the more present component. To further expedite the simulation, a minimum delta temperature equal to 2 K is set under heading `Re-solve temperature`; this means that for temperature changes smaller than two degrees the rate coefficients are not recalculated, resulting in significant time savings. To further speed up the simulation, Converge includes the adaptive zoning, i.e. a tool that groups together cells with similar features (e.g. temperature and reaction ratio), allowing to apply the chemistry solver once per group rather than once per cell. In the present work, temperature and reaction ratio for adaptive zoning chemistry are set equal to 5 K and 0.05 respectively.

5.3 Firing cycle results

As reported in section 5.1.2, different gasoline surrogates are generated using the Morgan [31] and the Ghosh [58] methodologies, to identify the properties of the blend that gives results comparable to the experimental ones. Furthermore, a first simulation is performed with the same injected species and vapour species used in the spray calibration process. Compositions and properties are reported in tables 5.2 and 5.3.

<table>
<thead>
<tr>
<th>Species</th>
<th>Blend 1 [58]</th>
<th>Blend 2 [58]</th>
<th>Blend 3 [31]</th>
</tr>
</thead>
<tbody>
<tr>
<td>i-Octane (C8H18)</td>
<td>50%</td>
<td>32%</td>
<td>5.833%</td>
</tr>
<tr>
<td>n-Heptane (C7H16)</td>
<td>11%</td>
<td>14%</td>
<td>18.749%</td>
</tr>
<tr>
<td>Toluene (C7H8)</td>
<td>39%</td>
<td>54%</td>
<td>75.418%</td>
</tr>
</tbody>
</table>

Table 5.2: Composition of the surrogates injected fuel
Table 5.3: Properties of the surrogates injected fuel

<table>
<thead>
<tr>
<th>Properties</th>
<th>Target</th>
<th>C8H18</th>
<th>Blend 1 [58]</th>
<th>Blend 2 [58]</th>
<th>Blend 3 [31]</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>98</td>
<td>100</td>
<td>97.97</td>
<td>98.37</td>
<td>98.5</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
<td>42.63</td>
<td>44.75</td>
<td>43.11</td>
<td>42.55</td>
<td>42.81</td>
</tr>
<tr>
<td>$\alpha_{st}$</td>
<td>14.17</td>
<td>15.03</td>
<td>14.32</td>
<td>14.07</td>
<td>13.75</td>
</tr>
<tr>
<td>$\rho$</td>
<td>727</td>
<td>673.2</td>
<td>733.9</td>
<td>757.5</td>
<td>791</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>0.76</td>
<td>0.72</td>
<td>0.75</td>
<td>0.77</td>
<td>0.78</td>
</tr>
</tbody>
</table>

In tables 5.2 and 5.3, Blend 1 and Blend 2 are produced using the Ghosh methodology, while Blend 3 is already defined and experimentally validated in the Morgan work; this is the reason for which the in first two blends integer numbers are used to define the volume fractions of each component, whereas in the last one three decimal points are present. The values of density (defined at 330 K from the Converge liquid.dat) and LHV are evaluated as the weighted average based on the mass fraction of each component. The stoichiometric air to fuel ratio is evaluated considering the complete oxidation of a generic hydrocarbon fuel $C_aH_b$ in $H_2O$ and $CO_2$, for which the reaction reported in formula 5.20 can be written.

$$C_aH_b + \left( a + \frac{b}{4} \right) (O_2 + \phi N_2) \rightarrow aCO_2 + \frac{b}{2} H_2O + \phi \left( a + \frac{b}{4} \right) N_2$$

(5.20)

where $\phi$ is the average molecular ratio of $N_2$ and $O_2$ in the air ($\phi = 79/21$). From relation 5.20, the stoichiometric air to fuel ratio can be evaluated as

$$\lambda = \frac{(aC + \frac{bM}{2}) \cdot (M_{O_2} + \phi M_{N_2})}{aCM_C + bHM_H}$$

(5.21)

where letter $M$ indicates the molar mass ($M_C = 12,0107$ g/mol, $M_H = 1,00794$ g/mol, $M_N = 14$ g/mol, $M_O = 15,999$ g/mol).

To evaluate the value of $\lambda$, the actual air to fuel ratio is normalized with respect to the stoichiometric one.

$$\lambda = \frac{A/F}{(A/F)_{st}} = \frac{\alpha}{\alpha_{st}}$$

(5.22)

in which the air to fuel ratio $\alpha$ is computed as the ratio between the air mass flow rate $q_a$ and the fuel mass flow rate $q_f$ experimentally measured (equation 5.23).

$$\alpha = \frac{q_a}{q_f} = \frac{1908 \ [kg/h]}{177,2 \ [kg/h]} = 10.76$$

(5.23)

The simulation performed with CSL_Gasoline_v1 as injected species and i-octane as the single vapour species in which the liquid fuel can evaporate leads to a slow combustion and thus the peak pressure is lower than the expected one and shifted toward the expansion stroke. This behaviour is probably due to the low $\lambda$ value obtained considering only the i-octane as burning species; as a matter of fact, the computed $\lambda$ is equal to 0.72 and the mean $\lambda$ measured in the combustion chamber at the spark discharge event is equal to 0.81; this shift of $\lambda$ toward low values, i.e. toward an over-rich mixture makes the laminar burning speed and thus also the turbulent speed lower. Using Blend 1 and Blend 2, the pressure traces are almost equal; combustion occurs faster with respect to the reference and thus the peak pressure is higher and earlier. Finally, using the Blend 3 the pressure curve appears to be
more similar to the experimental one.

![Figure 5.4: Cylinder pressure as a function of the crank angle for Blend 1, Blend 2 and Blend 3](image)

However, from the Heat Release Rate (HRR) plots (figure 5.5), it can be seen that for all the four test cases, the start of combustion occurs in advance. Thus, the issue is the definition of the correct ignition timing.

![Figure 5.5: Heat Release Rate as a function of the crank angle for Blend 1, Blend 2 and Blend 3](image)

The spark timing was defined according to the calibration parameter set on the electronic control unit for this specific working point. From now on, the delay between the value imposed on the ECU and the actual event, due for example by the knock detection unit, is taken into account. Considering an engine speed equal to 7000 rpm, the delay that has to be subtracted from the imposed spark advance (SA) is 0.75 crank angles. Using the same energy shape defined in section 5.2.1 and a SA equal to 14.75 crank angles, instead of 15.50, surrogate Blend 3 is tested again; simulations performed with Blend 1 and Blend 2 are not tested again, since the slope and the peak value of both the HRR and of the pressure curve is too far from the expected one.

Moreover another blend is defined; as a matter of fact, the three blends are defined with an increasing volume fraction of toluene. Between the second and the third blend, a big step, from 54% to 75.5% can be observed. Thus a fourth surrogate with similar properties of the experimental gasoline and a toluene volume fraction in between these two values is tested; its composition and properties gathered through the Morgan methodology are reported in tables 5.4 and 5.5.
Species [Volume fraction] | Blend 4 [31]
--- | ---
i-Octane (C8H18) | 19% 
n-Heptane (C7H16) | 16% 
Toluene (C7H8) | 65% 

Table 5.4: Composition of the fourth surrogate

<table>
<thead>
<tr>
<th>Properties</th>
<th>Target</th>
<th>Blend 4 [31]</th>
</tr>
</thead>
<tbody>
<tr>
<td>RON</td>
<td>98</td>
<td>98.02</td>
</tr>
<tr>
<td>LHV [MJ/kg]</td>
<td>42.63</td>
<td>42.16</td>
</tr>
<tr>
<td>$\alpha_{st}$</td>
<td>14.17</td>
<td>13.91</td>
</tr>
<tr>
<td>$\rho$</td>
<td>727</td>
<td>774.9</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>0.76</td>
<td>0.77</td>
</tr>
</tbody>
</table>

Table 5.5: Properties of the fourth surrogate

As expected, reducing the spark advance causes a reduction of the pressure peak. For a wide interval of crank angle, the pressure trace is in between the maximum and minimum values obtained on the engine test rig and the peak pressure deviates of less than 1% with respect the target value. However, after having reached the maximum pressure value, combustion process continues faster with respect to the experimental data. This is clearly visible from the HRR plot (figure 5.7): up to the maximum value of HRR, the simulation results show an extremely good agreement with the experimental ones while, after this point the simulation curve is larger than the experimental one. This behaviour can be also related to a not perfect tuning of the heat transfer between the charge and the combustion chamber walls, for which a more complex model of the one used in this work, such as the mono-dimensional conjugate heat transfer, should be employed.

![Figure 5.6: Cylinder pressure as a function of the crank angle for Blend 3 and Blend 4](image-url)
Figure 5.7: Heat Release Rate as a function of the crank angle for Blend 3 and Blend 4

Regarding the Blend 4, it can be seen that a slower combustion and a lower peak pressure are obtained with respect to the simulation performed with the Blend 3; however, during the expansion stroke, the two pressure traces are almost superimposed, probably thanks to the lower heating value of the fourth blend. Results shown from now on are related to the simulation performed with the third blend, since among the different gasoline surrogates tested, shows the best agreement with the experimental data.

5.3.1 Equivalence ratio

The distribution of the fuel inside the combustion chamber heavily influences combustion and pollutant formation processes; as a matter of fact, the overall burning speed of a specific fuel and thus the combustion efficiency, is affected by the local equivalence ratio $\phi$; for standard gasoline, the maximum laminar flame speed is obtained for slightly rich mixture, with the equivalence ratio about 1.1 [62].

In direct injection engines, the reduced time available for the spray evaporation and spread through the combustion chamber, generates over rich and over lean regions; extremely fuel rich zones ($\phi > 2$), in addition to the reduction of the burning speed, lead to soot and unburned hydrocarbon (HC) formation due to wall quenching phenomena, while lean spots are responsible of HC emissions generated through bulk quenching.

Figure 5.8 shows the equivalence ratio in the cylinder at spark timing, i.e. 705 crank angles; it can be seen that the values of equivalence ratio range from 1.5 near the cylinder liner, to 0.7 near the injector tip. Close to the spark plug, the equivalence ratio is about 1.2 and in most of the plotted surfaces it is in between 1.2 and the stoichiometric value; as said before, these condition is the most suitable for having a fast combustion.

To have a more precise view of the equivalence ratio distribution inside the combustion chamber, the bar graph reporting the in cylinder fuel mass belonging to a specified equivalent ratio range can be reported (figure 5.9). As gathered from a qualitative point of view through figure 5.8, most of the mixture is stoichiometric or slightly rich; the mass of mixture characterized by an equivalence ratio below the range 0.7-0.8, is almost negligible, whereas about 7% of the overall mass has an equivalence ratio grater than 1.5.
5.3.2 Flame front development

As already mentioned, the in-cylinder turbulences have a large impact on the combustion processes; their intensity affect the propagation speed of the flame front, whereas their structure defines the predominant direction development of the flame. In figure 5.10 the in-cylinder temperature is reported as a function of the crank angle. The following aspects can be highlighted: throughout the entire combustion process, three main regions can be identified: the unburned region characterized by a temperature lower than 1000 K, the flame front layer, whose temperature is in between 1500 K and 2000 K and the burned region, where the highest temperatures are reached. As a matter of fact, the gas belonging to the regions in which combustion occurs earlier are further compressed after combustion reaching higher temperatures than the gas compressed before burning. The development of the flame front is not symmetrical with respect to the cylinder axis, but it is promoted toward the intake valve region.

The unbalance in the combustion process toward the intake side is the result of the in-
teraction between the organized in-cylinder motion and the flame front; figure 5.11 shows the motion patterns present in the cylinder at spark timing through a vectorial representation, along with the turbulent kinetic energy on the color scale. On the tumble plane, it can be highlighted a big vortex rotating in counterclockwise direction toward the intake side that originates from a strong velocity flow field positioned below the spark plug (figure 5.11a); this is responsible for the deviation of the flame front toward the intake valve region. From the top view (figure 5.11b), two main symmetrical vortices, one above the $xz$ plane passing through the cylinder axis and one below it, with a counterclockwise and a clockwise rotation respectively, can be highlighted. These increase the propagation of the flame front in the direction defined by the normal vector of the tumble plane (y direction).

![Figure 5.11](image)

Figure 5.11: Turbulent kinetic energy and velocity vectors at spark timing (705 °CA) on the tumble plane passing through the cylinder axis
Figure 5.10: In-cylinder temperature on the tumble plane passing through the cylinder axis (left column), on the swirl plane passing through the squish plane (right column). Sampling time: 5 °CA after SOC (a) and (b), 25 °CA after SOC (c) and (d), 45 °CA after SOC (e) and (f)
Chapter 6

Conclusions and future work

In this thesis, a numerical study on spray and combustion in a GDI engine, performed on the 3-D computational fluid dynamics software Converge (V2.4), is shown. The work was divided in two main sections: in the first one, a spray calibration procedure, based on experimental data, was performed in order to lay the basis for the next phase of the work, i.e. the combustion simulation on a specific point of the engine working map of the engine under study.

The spray calibration procedure consisted in the definition of the most suitable values of the parameters affecting the spray behaviour; this was done in order to have a spray with characteristics comparable to the real one, since in GDI engines, characterized by a reduced time for spray breakup and evaporation, droplets dimensions and spatial distribution heavily affect both the engine performances and the pollutant emissions. The spray calibration procedure was based on droplets speed, Sauter mean diameter and liquid length penetration experimentally measured in a quiescent constant volume cubic vessel; two operating conditions, defined in terms of injection pressure and chamber air temperature were tested, for which a single calibration procedure is carried on. This choice allowed to get a more stable and robust numerical model. Main results obtained during the spray calibration procedure are listed below:

- The definition of the convergent grid, i.e. the mesh refinement level below which a further refinement would have negligible effects on the simulation results, was the one defined as GRID 2, characterized by about 1 million of cells defined as reported in table 3.7.

- The discharge coefficient $C_d$ analytically evaluated, equal to 0.503, resulted to be the one able to better capture the trend of the experimental liquid length penetration.

- The calibration of the parameters (characteristic size and spread parameter) of the Rosin-Rammler distribution, according to which the size of the droplets exiting the nozzle is defined, led to a characteristic size equal to 27 $\mu m$ and to a spread parameter equal to 5.

- The value of the Rayleigh-Taylor size constant was equal to 0.6.

- For both the test conditions, extremely good liquid length penetrations and droplets velocity were obtained; the SMD resulted to be slightly overestimated in the first test condition. Moreover, numerical model turned out to be able to faithfully replicate the spray morphology throughout time.
The simulation of the cold cycle was performed to set the basis for the combustion process; simulation results are compared to results gathered from a validated GT-Power model. The most important results are reported in the following list:

- The model was able to correctly replicate the intake mass flow rate and thus the in-cylinder trapped mass; pressure and temperature traces faithfully followed the target values until the spark discharge event.

- The predominant in-cylinder pattern motion is a normal tumble, generated by the design of the combustion chamber and of the intake port. The turbulent kinetic energy at spark timing was higher near to the spark plug gap, if compared to the volume average in the whole cylinder, increasing the combustion velocity.

- The injection was defined to avoid spray-intake valve interaction; an overall rich mixture was obtained, with three rich spots ($\phi = 1.5$) near the cylinder liner.

Finally, the combustion model was added to the numerical model. The SAGE detailed chemical kinetics solver was chosen to simulate the oxidation reactions. Four surrogates, defined with ON, LHV and $\alpha_{st}$ similar to the experimental gasoline, were defined and tested.

- The surrogate defined as Blend 3 in table 5.2 showed the best match with the experimental pressure and HRR traces.

- Turbulences and air motion near the spark plug had a strong influence on the development of the flame front, for what concerns both velocity and direction.

This thesis research could be the basis for further development; possible suggestions are:

- Testing the fuel surrogate along with the combustion model against different operating conditions, to assess the sensitivity of the model.

- Add the emissions model, to investigate PM and HC emissions.

- Onset of knock is one of the most limiting obstacles for spark ignition engines. For this reason it could be useful to assess the capability of the model to replicate abnormal combustion phenomena.
Acknowledgements

I should first like to thank my supervisor Prof. Federico Millo, for the knowledge and the motivations he provided to me during both his study course and the thesis activity. Thank you for giving me the possibility of deepen this topic and for being my guidance on this important journey.

I would like to sincerely thank Andrea Piano, PhD and Prof. Luciano Rolando, who supported me in the daily work with persistence and commitment, always ready to help me with valuable advices and suggestions.

Furthermore, I would like to thank Dr. Stefano Paltrinieri, Dr. Fabio Berni and Ing. Fabio Santi Mortellaro, who supported me providing data and information without which this work would not be possible.

I would like to sincerely thank all my friends, old and new, who spent with me precious time. A special thanks to my colleagues, who shared with me these years of study at the Politecnico di Torino. Thank you all for making this journey livelier.

A big thank you to my parents grandparents that, with their sweet and tireless support during all my educational life, allowed me to get here. Last but not least, a huge thanks to my sister Elena, that represents for me an example of dedication to follow.
Bibliography


