1 Introduction

All over the world, Diesel engines are in use for power generation and transport with great success. One of the major benefits of the Diesel engine is its efficient energy conversion and high volumetric energy density. High torque at low speed was always a benefit of the Diesel engine for heavy duty applications. For passenger car applications the introduction of the turbo-charger and the direct injection system has released an increase of market shares more than 50% in Europe.

A major disadvantage are nevertheless the emissions formation. Particularly the particulates matter (PM) which consists mostly of soot, and NO_x emissions are subject of the emissions legislations. The emission regulations in the United States of America, Tier 2 / Bin 5 in 2007 and 2010, and in Europe, EURO 5 in 2010 and EURO 6 in 2014, request high challenges for all automotive companies and suppliers. The Diesel engine combustion has to become cleaner everbefore. Solutions for a clean combustion in the Diesel engine foresee a combination of lowered compression ratios, higher boost pressures, cooled EGR on the low- and high pressure side and new combustion concepts, e.g. the use of an early fuel injection strategy for a concept denoted as Premixed Charge Compression Ignition (PCCI).

Conventional combustion and advanced combustion modes are to be evaluated at different loads and speeds to find an optimal point with low engine-out emissions. This calibration work is usually a quite time consuming and cost intensive process. Computational Aided Engineering (CAE) offers here a solution to reduce these costs and shorten the development time. A virtual engine design can evaluate different bowl designs for a wide range of operating points and find optimal parameters much faster. However, this approach assumes that the underlying models for mixture formation, combustion and pollutant formation are physically well based and predictive.

It is therefore the objective of this thesis to study the spray and mixture formation

in Diesel sprays and the ongoing combustion process in Diesel engines by means of computational fluid dynamics (CFD). An optimization procedure is carried out to adjust unknown spray model parameters, denoted as spray model calibration. The same adjustment of spray model parameters can be achieved by applying a Genetic Algorithm if spray data is available. However for most engines, spray data is not available and only pressure trace and engine-out emissions are provided. In that case, a methodology has been developed by which the model is calibrated. Furthermore, validation is required to quote if the model can predict combustion and emissions in Diesel engines.

The thesis will first present the models that are applied in the engine simulation. The flow simulation is based on the numerical solution of the Favre-averaged Navier-Stokes equations for an incompressible fluid. The used spray model with sub-models accounting for droplet-breakup, droplet collision and coalescence, and droplet evaporation is reviewed in detail in chapter 3. The flamelet model approach is used as combustion model in this work. This approach includes models for pollutant formation as well. Both models are presented in chapter 4. Two different studies of the mixture formation in diesel fuel and ethanol spray are presented in chapter 5. The simulation results are compared with measured spray penetration data and results from PDA and Raman measurements. The spray model parameters are optimized by a Genetic Algorithm. This algorithm is suitable to find an agreement between simulation and experiment. Furthermore a simulation of two different engines is presented in chapter 6. In these engine cases, no spray data is available and an a-priori spray calibration cannot be conducted. Instead, a methodology to adjust the spray parameters is introduced. Conventional and PCCI combustion modes are investigated and the prediction of the model is validated. Finally, the results of the thesis are summarized in chapter 7.

2 Fluid Dynamics

It was Claude Louis Marie Henri Navier in 1821 and 1822 in France and George Gabriel Stokes in 1842 and 1843 in England who independently derived equations to describe the motion of fluids for an inviscous fluid similar to an elastic solid. Later this model was extended to a viscous fluid.
Today, the Navier-Stokes equations are widely applied in engineering. An analytical solution is obtained only in a limited number of problems. For practical applications, the Navier-Stokes equations are usually solved numerically. This approach has become very attractive with the on-going development of computer ressources although even today, the mathematical fundamentals of the Navier-Stokes equations are unclear as Feffermann claims [52] and included in a collection of unsolved mathematical problems [89].

2.1 Conservation Equations in Fluid Dynamics

In classical mechanics, conservation laws are familiar and derived for a control mass Ω_{CM}. In fluids, no fixed control mass exist since the fluid is streaming. Instead of a control mass, a control volume Ω_{CV} is introduced as a fixed spatial region in which the fluid flows. Within a discrete time between t_1 and t_2, the fluid is entering and leaving that control volume over its control surface S_{CV}. As in classical mechanics, mass m, momentum $\boldsymbol{I} = m \cdot \boldsymbol{u}$ and energy E have to be conserved. Similar as in thermodynamics, intensive properties are introduced, namely the density ρ, momentum per unit mass, namely the velocity $\boldsymbol{u}$, and energy per unit mass e. The fluid is assumed to be a continuous medium. Macroscopic intensive properties are obtained from the statistical average state of the molecules' microscopic properties. It is required that

the smallest dimension of the problem and the appropriate control volume are larger than the molecules' mean free path. Thus, the mean density of a fluid is defined as

$$\rho = \lim_{\delta V \to \delta V'} \frac{\delta m}{\delta V} \tag{2.1}$$

where δm is an infinitesimal mass of an infinitesimal volume δV which cannot be smaller than the smallest volume $\delta V'$ which is the lowest limit of a continuous fluid. Then, any extensive property $\boldsymbol{\Phi}$ is related to its intensive property $\boldsymbol{\phi}$ by the following integral over the volume Ω_{CM} that includes the control mass

$$\boldsymbol{\Phi} = \int\limits_{\Omega_{\mathrm{CM}}} \rho \boldsymbol{\phi} \mathrm{d}\Omega \, , \boldsymbol{\Phi} = \begin{pmatrix} m \\ \boldsymbol{I} \\ E \end{pmatrix} \, , \boldsymbol{\phi} = \begin{pmatrix} 1 \\ \boldsymbol{u} \\ e \end{pmatrix} \, . \tag{2.2}$$

The specific energy e is here the sum of inner energy u, potential and kinetic energy. The density ρ as well as the extensive and intensive properties $\boldsymbol{\Phi}$ and $\boldsymbol{\phi}$, respectively, are field functions and depend on the point $\boldsymbol{x}$ in space and time t:

$$\boldsymbol{\phi} = \boldsymbol{\phi}(\boldsymbol{x}, t) \tag{2.3}$$

By applying a time-derivative operator on Eq. (2.2), one yields the control volume equation also denoted as Reynolds' transport theorem [149]

$$\frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_{\mathrm{CM}}} \rho \boldsymbol{\phi} \mathrm{d}\Omega = \frac{\mathrm{d}}{\mathrm{d}t} \int\limits_{\Omega_{\mathrm{CV}}} \rho \boldsymbol{\phi} \mathrm{d}\Omega + \int\limits_{S_{\mathrm{CV}}} \rho \boldsymbol{\phi} \left(\boldsymbol{u} - \boldsymbol{u}_b \right) \cdot \boldsymbol{n} \mathrm{d}S \, , \tag{2.4}$$

where $\boldsymbol{n}$ the normal unit vector that points outwards, $\boldsymbol{u}$ is the velocity vector and $\boldsymbol{u}_b$ is the velocity of a moving control surface. For short, $\Omega = \Omega_{\mathrm{CV}}$ and $S = S_{\mathrm{CV}}$ will be used further on. Most applications have a fixed control volume so that $\boldsymbol{u}_b$ becomes zero but in engine cases, the motion of the piston and valves has to be addressed.
The Reynolds' transport theorem Eq. (2.4) is a balance equation. The rate of change of a property $\boldsymbol{\Phi}$ of the control mass is equal to the rate of change of the property in the control volume plus the net rate flux over the surface. That flux is caused by the motion of the fluid relative to the boundary and is denoted as convective flux. From Eq. (2.4), the integral form of mass conservation which is the continuity equation,

momentum conservation equation and energy conservation equation are derived:

$$\text{continuity} \quad : \quad \frac{\partial}{\partial t}\int\limits_{\Omega} \rho \mathrm{d}\Omega + \int\limits_{S} \rho \boldsymbol{u} \cdot \boldsymbol{n} \mathrm{d}S = \rho \dot{S} \tag{2.5}$$

$$\text{momentum} \quad : \quad \frac{\partial}{\partial t}\int\limits_{\Omega} \rho \boldsymbol{u} \mathrm{d}\Omega + \int\limits_{S} \rho \boldsymbol{u}\boldsymbol{u} \cdot \boldsymbol{n} \mathrm{d}S = \sum \boldsymbol{F} \tag{2.6}$$

$$\text{energy} \quad : \quad \frac{\partial}{\partial t}\int\limits_{\Omega} \rho e \mathrm{d}\Omega + \int\limits_{S} \rho e \boldsymbol{u} \cdot \boldsymbol{n} \mathrm{d}S = \sum \dot{Q} \tag{2.7}$$

In Eq. (2.6) and Eq. (2.7), the source term on the right hand side $\sum \boldsymbol{F}$ and $\sum \dot{Q}$ are the forces and energy sources whereas source terms $\dot{S}$ in the continuity equation Eq. (2.5) are only due to the phase-transition from liquid to gas phase.
The main forces that act on a fluid are surface and body forces. Surface forces are due to pressure gradients, normal and shear stresses. Body forces include gravity, centrifugal and Coriolis forces. Here, only gravity force is considered as body force. The gravity forces addresses buoyancy effects but is neglected. Surface forces are induced by pressure forces and by stresses on a micro-molecular level. These have to be correlated to macro-molecular properties such as pressure and velocity by making assumptions. A very popular approach is to assume a Newtonian fluid in which the stress is proportional to the velocity gradient. The molecular rate of momentum transport is expressed by the viscous stress tensor $\boldsymbol{T}$

$$\boldsymbol{T} = -\left(p + \frac{2}{3}\mu \nabla \cdot \boldsymbol{u}\right)\boldsymbol{I} + 2\mu \boldsymbol{S} \tag{2.8}$$

where $\boldsymbol{I}$ is the unit tensor and $\boldsymbol{S}$ the strain-rate tensor

$$\boldsymbol{S} = \frac{1}{2}\left[\nabla \boldsymbol{u} + (\nabla \boldsymbol{u})^T\right] \ . \tag{2.9}$$

In Einstein notation, these equations are rewritten as

$$T_{ij} = -\left(p + \frac{2}{3}\mu \frac{\partial u_j}{\partial x_j}\right)\delta_{ij} + 2\mu S_{ij} \tag{2.10}$$

and

$$S_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \ . \tag{2.11}$$