1 Introduction

For the conversion of chemical energy to thermal energy to mechanical energy, combustion represents up to now the most important process with fossil fuels being the most important source of energy. The internal combustion (IC) engine has been developed in the late 19^{th} century, and regarding fuel efficiency, economy, and emissions the device has been significantly improved since. Although many alternative concepts like electrical or hybrid power trains or fuel cells are investigated and developed, the dominant device in the near and intermediate future is expected to be the IC-engine.

Over the past decades, one of the major drivers for the improvement and optimisation of the IC engine has been the enforcement of stricter emission regulations in the US as well as in Europe and in Japan. To be able to achieve the legislative restrictions new technologies and especially new combustion concepts have been developed. On the aftertreatment side the development of catalyst systems and particle filters have significantly reduced the output of emissions. However the improvement lead to a decrease in fuel efficiency and actually does not address the cause of the emissions. For the fulfillment of future requirements concerning fuel consumption and emission standards, two combustion concepts are considered as being the most promising approach: turbo-charged diesel and stratified spark ignition (SI) engines with high pressure direct injection (DI) systems.

While DISI-engine are supposed to have a much higher potential in terms of fuel consumption economy compared to the classical homogeneous combustion concepts, combustion stability and emission are the major topics of concern. Cyclic variability represents a critical issue in DISI-engines, as cycle-to-cycle variations are substantial to the combustibility of the air/fuel mixture at the time of the discharge of the spark plug leading to partial burning or even misfire. These incomplete combustion cycles lead to a significant increase in emissions, especially unburned hydrocarbon emissions, and a significant reduction in terms of fuel efficiency, therefore rendering it highly undesirable. Thus the cycle-to-cycle variations of the gas motion have been identified as playing a key role for the further optimisation of combustion process and thus the complete device. While the impact onto the combustion process is immediately visible, the cause for the cyclic variability is not yet fully understood, although generally attributed to turbulence effects.

Computational fluid dynamics (CFD) in combination with Reynolds averaged Navier-Stokes (RANS) turbulence modeling closures has been established as a very efficient and reliable tool for the description and analysis of the flow and combustion processes inside IC engine. Additionally, the application of CFD allows insights into various physical processes which are difficult to study experimentally. Even further, in the design and development process in an industrial context, CFD is applied for instance in the optimization of intake and engine geometries, leading to a significant reduction of development

cost as well as turnaround time. Based on common Reynolds averaged Navier-Stokes (RANS) turbulence modeling, this approach is by definition limited to the description of (statistical) mean values. In case highly transient and unsteady features such as cycle-to-cycle variations are investigated, this approach is not capable to capture this kind of phenomenon.

The ability to predict cyclic variations is given by the alternative turbulence modelling approach, namely large eddy simulation (LES)[1]. In contrast to the statistical approach of RANS, the LES approach describes the filtered turbulent flow field, i.e. a significant amount of the turbulent spectrum is resolved and a smaller range of turbulent length scales needs to be modeled. The numerical cost however, caused by resolving smaller temporal and spatial scales, requires higher-order numerical schemes, smaller time steps and higher resolutions of the computational grids, lead to a significant increase of CPU-time and memory consumption compared to RANS.

An alternative modelling approach is the combination of both models in a hybrid RANS/LES approach, obtaining the attractive features of both methods. These methods provide the opportunity to use LES in regions, where its performance is known to be essentially superior to RANS. In other regions, where the accuracy and the averaged information on turbulent properties is sufficient, RANS can be used in order to save CPU-time. In contrast to pure RANS temporal fluctuations can be resolved in the LES regions in hybrid methods giving these approaches the potential to predict cycle-to-cycle variations or other turbulent flows of highly unsteady nature.

The structure of the work is as follows. A summary of the governing equations for chemically reacting flows in given in chapter 2. Chapter 3 presents an introduction to turbulence and turbulence modelling. The statistical approach based on Reynolds averaging is introduced in 3.2, where also an overview of RANS models and model hierarchy in given. The LES technique based on a filtering approach as well as popular LES models are discussed in section 3.4, followed by he motivation for hybrid approaches combining elements of both RANS and LES and a discussion of hybrid models in section 3.5. In section 3.5.2 a new hybrid two-scale VLES model is presented. The chapter closes with a discussion of methods for the generation of turbulent initial and boundary conditions (artificial turbulence), section 3.6. Chapter 4 gives an overview of premixed laminar and turbulent combustion in sections 4.1 and 4.2. Additionally modelling approaches for turbulent premixed combustion in the RANS context based on the progress variable 4.3 and on a level set approach (G-equation) 4.4 are discussed as well as combustion modelling in the LES context with an overview of LES-based combustion models for pre-mixed turbulent combustion. The adaptation of the G-equation to the hybrid two-scale VLES approach finalises the chapter. The numerics of the CFD solver employed in this work are presented in section 5. The application, evaluation and discussion of the developed techniques and modelling approaches is done in chapter 6, starting with an analysis of

[1]The application of direct numerical simulation (DNS) is not considered as an option in terms of industrial applicability.

initialisation methods and influence of numerical schemes on the turbulent spectra in homogeneous, isotropic turbulence 6.1. The results of the simulation of a simplified engine configuration and multi-cycle simulation of a 4-valve model engine are discussed in sections 6.2 and 6.3 respectively. In order to demonstrate the feasibility to describe the effects of turbulence onto the flame propagation, the chapter closes with the numerical study of flame propagation in cylindrical vessel under high swirl condition 6.4. Summary and conclusions are given in chapter 7.

2 Physics of fluids

2.1 Fundamental equations of fluid mechanics

The description of fluid flow is based on equations describing the conservation of mass, momentum and energy. Considering the fluid as a continuum leads to the fundamental transport equation of fluid mechanics, the Navier-Stokes equation[1].

For compressible fluids in Cartesian coordinates the continuity equation, i.e. the conservation of mass, reads

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho U_i\right) = 0\,, \tag{2.1}$$

where ρ denotes the fluid density and U_i the x_i–velocity component. The conservation of momentum is described by

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial}{\partial x_j}\left(\rho U_i U_j\right) = -\frac{\partial p}{\partial x_i} + \frac{\partial \sigma_{ij}}{\partial x_j} + \rho g_i \tag{2.2}$$

with the viscous shear stress tensor σ_{ij} described by the Stokes relation

$$\sigma_{ij} \;=\; \mu \underbrace{\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right)}_{2\,S_{ij}} - \frac{2}{3}\mu \frac{\partial U_k}{\partial x_k}\delta_{ij} \tag{2.3}$$

p denotes the pressure and g_i represents external body forces per unit mass, as for instance gravitational acceleration. The rate of strain tensor S_{ij} is defined as

$$S_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) \tag{2.4}$$

A modified definition is usually employed for compressible flows in which the trace of the tensor is zero:

$$S^*_{ij} = \frac{1}{2}\left(\frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i}\right) - \frac{1}{3}\delta_{ij}\frac{\partial U_k}{\partial x_k}\,. \tag{2.5}$$

Using equation (2.5) the viscous shear stress tensor σ_{ij} can also be written in compact form as $\sigma_{ij} = 2\,\mu\, S^*_{ij}$. The transport equation for the total enthalpy h and species mass fraction Y_α read

$$\frac{\partial \rho h}{\partial t} + \frac{\partial \rho U_i h}{\partial x_i} = \frac{\partial p}{\partial t} + U_j \frac{\partial p}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial x_j}\right) + \sigma_{ij}\frac{\partial U_i}{\partial x_j} \tag{2.6}$$

$$\frac{\partial \rho Y_\alpha}{\partial t} + \frac{\partial \rho U_i Y_\alpha}{\partial x_i} = \frac{\partial}{\partial x_i}\left(\frac{\mu}{Sc_\alpha}\frac{\partial Y_i}{\partial x_i}\right) + \dot{\omega}_\alpha \tag{2.7}$$

[1] C.L.M.H. Navier was the first to derive these equations in 1823 despite his lack of understanding the full physics; in 1845 G.G. Stokes was the first to obtain a rigorous derivation of the Navier-Stokes equations.

where the diffusive transport in both equations is modelled using a gradient approach, namely Fourier's law for the enthalpy equation and Fick's law for the species mass fraction

$$J_i^\alpha = -\frac{\mu}{Sc_\alpha}\frac{\partial Y_\alpha}{\partial x_i}\,. \tag{2.8}$$

Sc_α denotes the Schmidt number, relating the diffusive transport of mass fractions to the dynamic viscosity. Note that equation (2.6) does not contain any source terms due to chemical reaction, since the total enthalpy h includes the chemical heat of formation.

The only terms which needs closure in equation (2.7) are the chemical reaction rates $\dot{\omega}_\alpha$. Each reaction rate contains the rates of progress τ_r of any elementary reaction r multiplied by the stoichiometric coefficient ν of species α in that reaction:

$$\dot{\omega}_\alpha = \sum_r \nu_{\alpha r}\tau_t = \sum_r \left(\nu_{\alpha r}^b - \nu_{\alpha r}^f\right)\tau_r\,. \tag{2.9}$$

The rate of progress is given by the forward (f) and backward (b) rate constants K_r and the product of the molar concentrations $[X]_\beta$ of the educt species:

$$\tau_r = K_r^f \prod_\beta [X]_\beta^{\nu_{\alpha\beta}^f} - K_r^b \prod_\beta [X]_\beta^{\nu_{\alpha\beta}^b}\,. \tag{2.10}$$

where the forward rate constants are usually modelled by a generalised Arrhenius approach

$$K_r^f = A_r T^{n_r} \exp\left(-\frac{E_r}{R_m T}\right)\,, \tag{2.11}$$

while in most cases the backward reaction is linked to K_r^f by the equilibrium constant $K_{c,r}$ via

$$K_{c,r} = \frac{K_r^f}{K_r^b}\,. \tag{2.12}$$

Further details can be found in the standard literature, for example [36]. The link between pressure, temperature, species distribution and density is done by means of the ideal gas law

$$\frac{p}{\rho} = \sum_\alpha \frac{Y_\alpha}{W_\alpha}\mathcal{R}T\,, \tag{2.13}$$

where $\mathcal{R}$ is the ideal gas constant and W_α the molecular weight of species α. Using the mean molecular weight W defined as

$$W = \left(\sum_\alpha \frac{Y_\alpha}{W_\alpha}\right)^{-1}\,, \tag{2.14}$$

equation (2.13) reduces to

$$p = \frac{\rho}{W}\mathcal{R}T\,, \tag{2.15}$$

2.2 Non-dimensional form

While for practical applications the dimensional form of the governing equation as given in the previous section is employed, the dimensionless variant is of importance for theoretical and fundamental studies. The non-dimensional variables are obtained by normalisation of the independent and dependent variables by reference values (indicated by the index R)

$$x_i^* = \frac{x_i}{l_R}, t^* = \frac{t \cdot U_R}{l_R};$$

$$\rho^* = \frac{\rho}{\rho_R}, U_i^* = \frac{U_i}{U_R}, p^* = \frac{p}{\rho_R U_R^2}, T^* = \frac{T}{T_R};$$

here, l_R, U_R, ρ_R and T_R represent a reference length, velocity, density and temperature respectively. Additional reference quantities required for the normalisation of the governing equations are the reference speed of sound c_R, the reference specific heat capacity at constant pressure c_{pR}, the reference dynamic viscosity μ_R, and finally the reference heat conductivity λ_R. Introducing the normalised variables into the governing equations (2.1), (2.2) and (2.6), and dropping the superscripts the following set of equations is obtained[2]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho U_i) = 0, \tag{2.16}$$

$$\frac{\partial \rho U_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho U_i U_j) = -\frac{\partial p}{\partial x_i} + \frac{1}{Re}\frac{\partial \sigma_{ij}}{\partial x_j}, \tag{2.17}$$

$$\begin{aligned} \frac{\partial \rho h}{\partial t} + \frac{\partial \rho U_i h}{\partial x_i} &= Ma^2 \frac{\partial p}{\partial t} + Ma^2 U_j \frac{\partial p}{\partial x_j} \\ &\quad + \frac{1}{Pr\, Re}\frac{\partial}{\partial x_j}\left(\frac{\lambda}{c_p}\frac{\partial h}{\partial x_j}\right) + \frac{Ma^2}{Re}\sigma_{ij}\frac{\partial U_i}{\partial x_j}. \end{aligned} \tag{2.18}$$

In the non-dimensional from of the conservations equation three characteristic numbers appear, namely the Reynolds number Re, the Mach number Ma, and the Prandtl number Pr, which are defined as

$$Re = \frac{\rho\, l\, u}{\mu} = \frac{l\, u}{\nu}, \; Ma = \frac{u}{c}, \; Pr = \frac{c_p\, \mu}{\lambda}, \tag{2.19}$$

where the index R indicating reference quantities has been omitted for brevity. These non-dimensional numbers allow to characterise and to classify the state of flow.

The Mach number Ma, defined as the ratio of the fluid velocity u to the (local) speed of sound c, see equation (2.19), is a measure for the compressibility of the flow. For small

[2]Here, the external body forces have been omitted for brevity.

model air plane	$l = 1\,m\,, u = 1\,m/s$	$Re = 7 \cdot 10^4$
cars	$u = 3\,m/s$	$Re = 6 \cdot 10^5$
air planes	$u = 30\,m/s$	$Re = 2 \cdot 10^7$
atmospheric flows		$Re \approx 7 \cdot 10^{20}$
internal combustion engine		$Re = 6 \cdot 10^4$

Table 2.1: Sample of characteristic Reynolds numbers.

Ma-numbers ($Ma < 0.3$), the flow can be considered as incompressible, which implies that the enthalpy equation is decoupled from the momentum and continuity equations. This effect can be seen in the enthalpy equation (2.18), considering the limit $Ma \to 0$, as in this limit, the enthalpy becomes independent of pressure.

The Reynolds number Re represents the ratio of inertia to viscous forces and is the most important dimensionless number in fluid dynamics. By means of the Reynolds number a criterion for determining the state of a fluid flow (laminar/turbulent) can be derived. Qualitatively speaking laminar flow occurs at low Reynolds numbers where viscous forces are dominant, while turbulent flow occurs at high Reynolds numbers, at which the inertia forces dominate the fluid motion. In table 2.1 typical values of the Re number for some aerodynamic flows are given.

For gaseous fluids the Prandtl-number Pr is of the order of unity.