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INTRODUCTION

Turbocharged direct injection spark ignition (DISI) engines represent a major step in the evolution of gasoline engines. DISI engines have become increasingly popular due to the potential to significantly improve fuel efficiency and emission levels while the performance of the engine is maintained or even enhanced. In turbocharged DISI engines, both the compression ratio and spark timing are limited by the occurrence of knock. Hence, it limits the thermodynamic efficiency and the performance of the engine. Engine knock is an irregular combustion phenomenon, which is promoted by autoignition processes in the unburnt gas ahead of the flame front. This phenomenon is a fundamental issue of modern spark ignition (SI) engines. Another important aspect is the formation of pollutants, such as nitrogen oxides (NOx) and soot. With the introduction of the stringent emission standard EURO 6 in 2014, these pollutants have to be considerably reduced compared to EURO 5. The new standard also limits the number of soot particles for the first time. Hence, the emissions of pollutants and the onset of knock are crucial criteria for the development of internal combustion (IC) engines. A more complete understanding of these physical processes can be obtained by combining experimental and numerical development tools. Especially the numerical simulation of the in-cylinder flow gives a deeper insight and enables a better understanding of the inherent physical phenomena. This makes it possible to improve and optimize the combustion process in IC engines.

Computational fluid dynamics (CFD) in combination with Reynolds-averaged Navier-Stokes (RANS) turbulence closures has been established as an efficient tool for the description and analysis of the flow inside IC engines. However, the three-dimensional simulation of turbulent reacting flows in internal combustion engines still represents one of the most challenging applications of computational fluid dynamics. A common approach to model turbulent reacting flows is to incorporate detailed chemical kinetics in order to determine the chemical source terms in the species transport equations. The use of finite-rate chemistry in computational fluid dynamics gives rise to a large system of nonlinear ordinary differential equations (ODE) for each computational cell, which leads to a dramatically increase in computational time. Despite the use of large chemical reaction mechanisms being limited by the computational power, the major challenge is still the description of turbulence chemistry interaction. In applications like IC engines, the fluctuations of temperature and species concentrations directly affect the chemical production rates. The difficulty lies in the accurate prediction of the mean chemical source term. This is especially true if the time scales of turbulence and chemical reactions are of the same order of magnitude. Hence, for the prediction of combustion, engine knock, and pollutant formation soundly based physical models are needed in the framework of a comprehensive engine simulation methodology.

In the gasoline engine development process at BMW, the commercial 3D-CFD solver ANSYS CFX is employed for the simulation of the in-cylinder flow in turbocharged DISI engines. The objective of this thesis was to enable the CFD code to correctly describe the turbulent flame front propagation, heat release, nitric oxide formation, and engine knock in turbocharged DISI engines. Special emphasis was put on the development of a simulation methodology that is able to predict these physical processes with high accuracy and without tuning parameters. In order to meet these demands, it was necessary to derive new physical models and to implement these into ANSYS CFX.

For the modeling of the turbulent combustion process the G-equation model was implemented in cooperation with ANSYS into the 3D-CFD solver ANSYS CFX. The G-equation is a level-set based flamelet model, originally proposed by Williams [123] and widely elaborated by Peters [80], Peters [82], and Peters [83]. It has proven in recent years to be successful in predicting the combustion process in spark ignition engines. The G-equation model provides a kinematic and geometrical description of the flame front, and there is no need for a source term closure. The major advantage of this combustion model is that the model constants are well-defined. Hence, it is not necessary to adjust the constants to fit experimental data, which considerably improves the predictability of the combustion simulation.

In order to incorporate detailed chemical kinetics into the in-cylinder flow simulation of IC engines, a multizone approach was employed. In the multizone approach the combustion chamber is split into several zones that are treated as homogeneous reactors. In each of these zones detailed chemistry is applied and solved in an external multizone chemistry solver. The multizone approach has demonstrated to accurately predict pressure traces and heat release rates in homogeneous charge compression ignition (HCCI) engines with a very low computational overhead. Despite the various existing multizone models having shown to produce reasonable results, they are lacking a sound mathematical and physical basis. The definition of a reactor and its interaction with other reactors within the multizone approach is rather vague. Since a sound mathematical and physical basis is missing, the interpretation of the results can become difficult because the underlying limitations of the employed approach are not clear. Hence, in the framework of this thesis a thorough derivation of the multizone approach is given. The derivation of the multizone approach is based on the conditional moment closure (CMC) equations proposed by Klimenko and Bilger [52]. This leads to the novel concept of the conditional multizone (CMZ) model. Based on this detailed derivation it is possible to deduce precise consequences regarding the modeling of reactors in phase space, e.g. how to determine the rate at which each reactor exchanges mass, heat, and species. Moreover, the novel multizone approach can also be conditioned on burnt and unburnt gases. By combining the multizone model with a turbulent combustion model for premixed flames, it can be used to predict both volumetric and front-like combustion modes and nitric oxide formation in SI engines.

Based on the conditional multizone approach, a model was derived to simulate the nitric oxide formation in turbocharged DISI engines. It is used in combination with the level-set based flamelet model. The combustion model is employed to simulate the overall heat release, whereas the multizone model is used to determine the chemical reactions in the post-flame region. The entire post-flame region is discretized by a small number of zero-dimensional well-stirred reactors. Within the reactors detailed chemical kinetics are used to model the slow process of nitric oxide formation. In order to solve the large system of nonlinear ordinary differential equations that result from the employed multizone model, a chemistry solver was developed. The multizone chemistry solver is interactively coupled with ANSYS CFX via Fortran user routines.

Engine knock is a very complex phenomenon involving chemical processes in the unburnt mixture, turbulent flame propagation, and detonation waves. Especially the erratic behavior and the impact of cycle-by-cycle variations makes the modeling of engine knock a challenging task. Most of the current modeling approaches do not provide statistical information regarding the formation of engine knock. They are solely based on mean quantities. Hence, they do not take into account the inherent feature of engine knock, namely that it is a stochastic phenomenon. In order to address the stochastic nature of engine knock, a generalized knock integral method was derived. This model solves a transport equation for the mean and the variance of a well-defined ignition progress variable. The chemical source term and the reaction term that appear in these balance equations are closed by employing a presumed PDF approach. Hence, the impact of mixture fraction and temperature fluctuations on the ignition progress variable is accounted for. The benefit of this generalized knock integral method is that it provides distinct criteria to determine the mean knock onset and to identify the locations of autoignition. Moreover, it also provides the probability of autoignition at every location in the combustion chamber.

The structure and outline of this work is as follows:

- Chapter 2 presents an introduction to turbulent flows. At first, the governing equations for chemically reacting flows are presented. This is followed by a phenomenological description of turbulence and a discussion of the basic concepts of probability theory. The Reynolds-averaged Navier-Stokes equations are introduced and complemented by an overview of different turbulent-viscosity models to determine the unclosed Reynolds stresses.

- An overview of the fundamentals of laminar and turbulent premixed combustion is given in Chapter 3. In the first part, the physics and structure of premixed laminar flames are discussed and the effects of strain and curvature on the flame structure are highlighted. This is followed by a description of the turbulence flame interaction. Finally, different modeling approaches for turbulent premixed combustion are presented.

- In Chapter 4, the implementation of the level-set based flamelet model for turbulent premixed combustion into ANSYS CFX is discussed in detail. The level-set approach for determining the flame front location is introduced, followed by the turbulence modeling of the G-equation. Subsequently, the integration of the combustion model into ANSYS CFX is outlined and the numerical treatment of the level-set approach is discussed. Finally, a thorough validation of the implemented level-set based flamelet model is presented.

- A detailed derivation of the novel conditional multizone approach is given in Chapter 5. At first, the conditional moment closure equations are extended to account for multiple conditions that are not restricted to conserved scalars. Based on these transport equations, a single conditional multizone model is derived, which can be applied e.g. to simulate the heat release in HCCI engines. In order to apply the multizone approach for SI engines, the model is extended to be used in combination with turbulent combustion models.

- Chapter 6 is devoted to new modeling approaches of engine knock and nitric oxide formation. The first part focuses on engine knock. A brief introduction on the nature of engine knock and an overview of current modeling approaches are given. This is followed by a description of the different stages of autoignition for a hydrocarbon fuel-air mixture. A novel knock model is proposed that can be interpreted as a generalized knock integral model. The second part is devoted to the modeling of nitric oxide formation. Based on the conditional multizone approach, a model is presented to simulate the nitric oxide formation in turbocharged DISI engines.

- The experimental and numerical settings are presented in Chapter 7. In the first part, the engine specifications and the measurement settings are introduced. This is followed by a description of the employed simulation approach, i.e. 1D gas dynamics coupled with a heat release analysis and 3D-CFD calculation.
- In Chapter 8, simulation results for a turbocharged DISI engine are presented and compared with experimental data. The gas exchange process, mixture formation, and combustion process are investigated for four different engine operating points. Special emphasis is put on the characterization of the interaction between turbulence and flame. The assessment of the nitric oxide model is based on a spark timing and equivalence ratio sweep. These sweeps were performed in order to evaluate the model's capacity to predict the impact of a variation in temperature and mixture composition on the formation of nitric oxide. Finally, simulation results of the knock model are presented. In order to validate the generalized knock model, a spark timing sweep was performed on the engine test bench for a full-load operating point. The simulation results are discussed in detail and are compared with experimental data.
- In the last chapter, a summary of the thesis work is given and areas for future work are highlighted.

2

DESCRIPTION OF TURBULENT FLOWS

The vast majority of the flows encountered in engineering practice are turbulent. All these turbulent flows share a common property: the ability to mix transported quantities much more quickly than the molecular diffusion processes. This is a very important characteristic feature of turbulent flows, since it has a direct impact on all practical applications. For instance, it increases the turbulent heat diffusion and the wall heat transfer, which is a crucial aspect for the design of heat exchange devices. Intake ports in turbocharged DISI engines are designed to produce high level of turbulence in order to enhance mixing between air and fuel in the combustion chamber. A high turbulence level also accelerates the combustion process. Without turbulence it would not be possible to operate an engine at high speeds, since the mixing and the combustion process would proceed too slowly. In addition, turbulence is highly dissipative and due to its erratic and chaotic behavior it can introduce flow instabilities that lead to a decrease in prediction accuracy. The underlying processes are very complex and different approaches as well as completely different points of view exist how to define turbulence. This chapter gives only a brief introduction to the physics of turbulence and to its modeling in the context of Reynolds-averaged Navier-Stokes (RANS) equations. For a comprehensive overview the reader is referred to Pope [93] and Lesieur [58].

In Section 2.1, the instantaneous conservation equations for reacting flows are presented. At first, the basic equations for describing the thermodynamical and chemical state of a reacting mixture are introduced. This is followed by a description of the governing equations of mass, species, momentum, and energy. Section 2.2 provides a short introduction to the nature of turbulence and a discussion of the characteristic scales of turbulent motion. It also introduces the basic concepts of probability theory, which is extensively used in this work. The Reynolds-averaged Navier-Stokes equations are presented in Section 2.3. Different turbulence models based on the turbulent-viscosity approach are discussed in order to provide closures for the unknown quantities in the averaged transport equations. Finally, a critical discussion of the RANS approach is given in Section 2.4.

2.1 GOVERNING EQUATIONS FOR REACTING FLOWS

2.1.1 *Thermochemistry and Chemical Kinetics*

A reacting mixture is composed of multiple species that can react chemically, which leads to a significant change in temperature and composition. Hence, the tracking of the thermodynamic state of a reacting mixture needs special attention. In the following, the basic equations for determining the state of a reacting mixture are presented.

Composition

There exist various ways or quantities to define the composition of a mixture. An overview of common quantities and useful relations is given in Table 2.1. In order to characterize the reacting mixture, the equivalence ratio ϕ is introduced. It is defined as the ratio of fuel mass fraction Y_F and oxidizer mass fraction Y_O normalized by the stoichiometric ratio $(Y_F/Y_O)_{st}$ (Poinsot and Veynante [90])

$$\phi = \left(\frac{Y_F}{Y_O}\right) \Big/ \left(\frac{Y_F}{Y_O}\right)_{st} . \tag{2.1}$$

The equivalence ratio is a central parameter for premixed combustion: rich combustion is obtained for $\phi > 1$ (the fuel is in excess), whereas lean combustion is characterized by $\phi < 1$ (the oxidizer is in excess). For non-premixed combustion, the mixture fraction Z is commonly used to characterize the composition of the reacting mixture (Peters [83]). Based on a two feed system with the fuel stream $\dot{m}_F$ and the oxidizer stream $\dot{m}_O$, the mixture fraction can be defined as the local ratio of the mass flux originating from the fuel stream to the total mass flux

Quantity	Definition
mass fraction Y_k	$Y_k = \frac{m_k}{m} = \frac{W_k}{W} X_k$
mole fraction X_k	$X_k = \frac{n_k}{n} = \frac{W}{W_k} Y_k$
partial density ρ_k	$\rho_k = \frac{m_k}{V}$
molar concentration $[X_k]$	$[X_k] = \frac{n_k}{V}$
mean molecular weight W	$W = \left(\sum_{k=1}^{N} \frac{Y_k}{W_k} \right)^{-1}$

Table 2.1: Definition of mass fraction, mole fraction, mass and molar concentrations as well as the mean molecular weight. m_k, n_k, V, W_k, and N denote mass, number of moles, volume, molecular weight, and number of species. The subscript k denotes the species index.

$$Z = \frac{\dot{m}_F}{\dot{m}_F + \dot{m}_O} . \tag{2.2}$$

The mixture fraction is related to the equivalence ratio according to

$$Z = \frac{\phi Z_{st}}{1 - Z_{st}(1-\phi)} \quad \text{and} \quad \phi = \frac{Z}{1-Z} \frac{1-Z_{st}}{Z_{st}} , \tag{2.3}$$

where the stoichiometric mixture fraction is denoted by Z_{st}.

Thermal Equation of State

The thermal equation of state provides the relationship between the pressure p, temperature T, and density ρ. For most technical applications, the law of ideal gases is reasonably accurate, which means that the intermolecular forces and the volume of the molecules can be neglected (Turns [118]). For a mixture of N perfect gases the pressure p, density ρ, and molar concentration $[X]$ are determined by

$$p = \sum_{k=1}^{N} p_k , \qquad \rho = \sum_{k=1}^{N} \rho_k , \text{ and} \qquad [X] = \sum_{k=1}^{N} [X_k] . \tag{2.4}$$

p_k, ρ_k, and $[X_k]$ are the corresponding partial quantities. The partial pressure is related to the concentration and temperature by

$$p_k = [X_k]\Re T = \frac{\rho_k}{W_k}\Re T\,, \tag{2.5}$$

where $\Re$ represents the universal gas constant and W_k is the molecular weight of species k. This leads to the well known equation of state for a mixture of N perfect gases

$$\frac{p}{\rho} = \sum_{k=1}^{N}\frac{Y_k}{W_k}\Re T = \frac{\Re}{W}T = R\,T\,. \tag{2.6}$$

The specific gas constant of the mixture is denoted by $R = \Re\,/\,W$.

As already stated above, the ideal gas assumption is only valid if the intermolecular forces can be neglected. Hence, at high pressures and high densities real gas effects need to be considered. Although the pressure in turbocharged SI engines can rise beyond 100 bar at full load, it is still reasonable to use the thermal equation for ideal gases. This is due to the fact that the pressure rise is caused mainly by the heat release during the combustion process. In this particular case, the density remains moderate due to the corresponding increase in temperature. However, for spray and wall film evaporation it can be necessary to account for real gas effects depending on the thermodynamic state of the multiphase flow, e.g. near the vapor-liquid critical point of the fluid.

Caloric Equations of State

In addition to the thermal equation of state $p = p(T, v)$, where $v = 1/\rho$ denotes the specific volume, it is also possible to define caloric equations of state given by

$$u_k = u_k(T, v) \quad \text{and} \quad h_k = h_k(T, p)\,. \tag{2.7}$$

These equations represent the general functional relationship of the internal energy u_k and the enthalpy h_k of species k with respect to the state variables T and v as well as T and p, respectively. It should be noted that other sets of variables, such as (p, v), could also be used to determine the caloric state of the mixture. The enthalpy is related to the internal energy via

$$h_k = u_k + p\,v\,. \tag{2.8}$$

The differential change of the internal energy and enthalpy can be obtained by differentiating Equation 2.7

$$\mathrm{d}u_k = \left(\frac{\partial u_k}{\partial T}\right)_v \mathrm{d}T + \left(\frac{\partial u_k}{\partial v}\right)_T \mathrm{d}v\,, \tag{2.9}$$

$$\mathrm{d}h_k = \left(\frac{\partial h_k}{\partial T}\right)_p \mathrm{d}T + \left(\frac{\partial h_k}{\partial p}\right)_T \mathrm{d}p\,. \tag{2.10}$$

It is known from kinetic gas theory that for an ideal gas the internal energy and the enthalpy are only functions of temperature. Hence, the partial derivatives with respect to the specific volume and pressure in Equation 2.9 and Equation 2.10 equal zero. By introducing the specific heat capacities at constant volume c_{vk} and constant pressure c_{pk}, it follows

$$\mathrm{d}u_k = \left(\frac{\partial u_k}{\partial T}\right)_v \mathrm{d}T = c_{vk}\,\mathrm{d}T\,, \tag{2.11}$$

$$\mathrm{d}h_k = \left(\frac{\partial h_k}{\partial T}\right)_p \mathrm{d}T = c_{pk}\,\mathrm{d}T\,. \tag{2.12}$$

The heat capacity simply defines the amount of heat which is needed to increase the temperature by one degree. The specific enthalpy h_k of species k is given by

$$h_k \;=\; h^0_{fk} + \int_{T_0}^{T} c_{pk}\,\mathrm{d}T\,, \tag{2.13}$$

where h^0_{fk} represents the standard enthalpy of formation at an arbitrarily chosen reference state (usually at the temperature $T_0 = 298.15$ K). The enthalpy h of the mixture is defined as the sum of the species enthalpies multiplied by their mass fractions

$$h \;=\; \sum_{k=1}^{N} h_k\,Y_k\,. \tag{2.14}$$

The mass specific heat capacity at constant pressure of the mixture is given by

$$c_p = \sum_{k=1}^{N} Y_k c_{pk}\,. \tag{2.15}$$

By combining Equations 2.13 and 2.14, the enthalpy of a reacting mixture can be written as

$$h \;=\; \underbrace{\int_{T_0}^{T} c_p\,\mathrm{d}T}_{\text{sensible}} + \underbrace{\sum_{k=1}^{N} h^0_{fk} Y_k}_{\text{chemical}}\;. \tag{2.16}$$

It shows that the mixture enthalpy h is a function of both temperature and composition. The first term on the right-hand side of Equation 2.16 is referred to as sensible enthalpy, whereas the second term is denoted as chemical enthalpy.

Chemical Kinetics

For a reacting mixture it is necessary to describe the change of its composition due to chemical reactions. The chemistry is usually described by a collection of elementary reactions (single step), which account for intermediate species and multiple transition states. A complete elementary reaction mechanism that accurately describes the chemistry of a certain fuel can consist of up to hundreds of species and even thousands of reactions for long-chain hydrocarbons (Curran et al. [20]). Hence, a compact mathematical notation is necessary to define a reaction mechanism. An outline of the commonly used notation is presented in the following.

Consider a reaction mechanism comprised of N species and M reactions

$$\sum_{k=1}^{N} \nu^f_{kj}\mathcal{M}_k \rightleftharpoons \sum_{k=1}^{N} \nu^r_{kj}\mathcal{M}_k \qquad j = 1,\ldots,M\,, \tag{2.17}$$

where $\mathcal{M}_k$ is the symbol for species k. The forward and reverse molar stoichiometric coefficients are denoted by ν^f_{kj} and ν^r_{kj}, respectively. The chemical source term $\dot{\omega}_k$ of species k reads

$$\dot{\omega}_k \;=\; W_k \sum_{j=1}^{M} \nu_{kj} w_j \quad \text{with} \quad \nu_{kj} = \nu^r_{kj} - \nu^f_{kj}\,. \tag{2.18}$$

w_j is the reaction rate of reaction j and can be expressed as

$$w_j \;=\; k_{fj} \prod_{k=1}^{N} [X_k]^{\nu^f_{kj}} - k_{rj} \prod_{k=1}^{N} [X_k]^{\nu^r_{kj}} \;. \tag{2.19}$$

The molar concentration of species k is denoted by $[X_k]$, and k_{fj} and k_{rj} are the forward and reverse reaction rate coefficients of reaction j. These reaction rates are usually modeled using the empirical *Arrhenius law* (Poinsot and Veynante [90])

$$k_j \;=\; A_j \, T^{\beta_j} \, \exp\left(-\frac{E_j}{\Re T}\right). \tag{2.20}$$

For each reaction j, values for the activation energy E_j, the temperature exponent β_j, and frequency factor A_j need to be provided.

2.1.2 *Conservation of Mass and Species*

The conservation equation of mass, also known as the continuity equation, is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho u_i) \;=\; 0 \,, \tag{2.21}$$

where ρ denotes the density, u_i the ith component of the velocity vector, t the time, and x_i the ith component of the Cartesian coordinate. The mass conservation equation is identical to the formulation for non-reacting flows. Although the total mass is conserved, the mass of each species varies due to chemical reactions. In order to account for the effects of chemical conversion, the mass conservation equation for each species k needs to be solved

$$\frac{\partial (\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_i} (\rho \, u_i \, Y_k) + \frac{\partial j_{ki}}{\partial x_i} \;=\; \dot{\omega}_k \quad \text{with} \quad k = 1, \ldots, N \,, \tag{2.22}$$

where Y_k is the mass fraction of species k, N the number of species, j_{ki} denotes the ith component of the diffusive flux of species k, and $\dot{\omega}_k$ is the reaction rate. In order to determine the source term $\dot{\omega}_k$, all chemical reactions in which species k takes part need to be evaluated. In contrast to the convective flux where the transport of a quantity is coupled to velocity, diffusive mass flux is provoked by gradients in the distribution of certain quantities such as temperature and species concentrations. The diffusive flux j_{ki} can be decomposed as follows

$$j_{ki} \;=\; j^c_{ki} + j^T_{ki} + j^p_{ki} \,, \tag{2.23}$$

where j^c_{ki} takes into account the mass flux associated with concentration gradients, whereas j^T_{ki} and j^p_{ki} denote the mass diffusion due to temperature and pressure gradients, respectively. j^p_{ki} can be neglected in internal combustion engines, since it becomes only important in cases of large pressure gradients. The second term on the right-hand side of Eq. 2.23 is associated with the *Soret-effect* (Warnatz et al. [122]). It accounts for the diffusive flux due to temperature gradients

$$j^T_{ki} \;=\; -\frac{D^T_k}{T} \frac{\partial T}{\partial x_i} \,. \tag{2.24}$$

The coefficient D^T_k denotes the diffusion coefficient of species k due to thermal diffusion. The *Soret-effect* leads to a mass flux of light molecules towards increasing temperature, whereas heavier molecules flow in the opposite direction. As a consequence, a concentration gradient within the mixture is established. The *Soret-effect* becomes important for light species and at low temperatures and, of course, at large temperature gradients (Warnatz et al. [122]). Hence, it should be considered in laminar diffusion flames, where cold unburnt gases are adjacent to hot burnt gases. In case of turbulent premixed flames, the temperature gradients are moderate because of the large flame thickness compared to a laminar flame; and it should be noted that the combustion in IC engines takes place at high temperatures. It is therefore reasonable and common to neglect the *Soret-effect* for the simulation of IC engines. The diffusive flux j^c_{ki} due to concentration gradients usually dominates the species diffusion process. In a multicomponent mixture consisting of N components, j^c_{ki} is defined by

$$j^c_{ki} \quad = \quad \frac{\rho W_k}{W^2} \sum_{\substack{l=1 \\ l \neq k}}^{N} D_{kl} W_l \frac{\partial X_l}{\partial x_i} \, , \tag{2.25}$$

where D_{kl} denotes the polynary diffusion coefficient of species k with respect to species l (Gerlinger [36]). W is the molecular weight of the mixture, and W_k and W_l denote the molecular weight of species k and l, respectively. The diffusion due to pressure and temperature gradients leads to segregation, whereas the diffusion associated with concentration gradients provokes a mass flux from regions of high to low concentrations. This leads to a homogenization of the species concentrations within a multicomponent mixture. Since most combustion processes occur in air and N_2 is abundant, all other species can be treated as trace species and D_{kl} can be approximated with $D_k = D_{kN_2}$. Based on Fick's law, the following approximation is commonly used (Peters [83])

$$j_{ki} = -\rho D_k \frac{\partial Y_k}{\partial x_i} \, . \tag{2.26}$$

Hence, by introducing the Schmidt number

$$Sc_k \quad = \quad \frac{\nu}{D_k} \, , \tag{2.27}$$

which compares the momentum and molecular diffusion of species k, the diffusive flux can be rewritten as

$$j_{ki} \quad = \quad -\frac{\mu}{Sc_k} \frac{\partial Y_k}{\partial x_i} \, . \tag{2.28}$$

Here, ν denotes the kinematic viscosity, which is related to the dynamic viscosity μ via $\nu = \mu / \rho$. It should be noted that this approximation violates mass conservation in a multicomponent system, since the sum of all N fluxes does not vanish. Therefore, it must not be used in laminar flame calculations (Peters [83]). For a detailed description of species diffusion processes the reader is referred to Bird et al. [9] and Hirschfelder et al. [45].

2.1.3 *Conservation of Momentum*

The conservation of momentum is described by

$$\frac{\partial \left(\rho u_j \right)}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho \, u_i \, u_j \right) \quad = \quad -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_i} \, , \tag{2.29}$$

where p denotes the static pressure and τ_{ij} the viscous stress tensor for a *Newtonian fluid*. Using Stokes' hypothesis, the stress tensor can be defined according to

$$\tau_{ij} \quad = \quad \mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}\right)-\frac{2}{3}\mu\frac{\partial u_k}{\partial x_k}\delta_{ij}\,. \tag{2.30}$$

δ_{ij} denotes the Kronecker symbol and μ represents the temperature-dependent dynamic viscosity. It is interesting to note that the momentum equation does not include explicit reaction terms and remains unchanged compared to non-reacting flows.

2.1.4 *Conservation of Energy*

The energy equation requires the greatest attention because multiple forms exist. The conservation equation for the enthalpy h is given by

$$\frac{\partial\left(\rho h\right)}{\partial t}+\frac{\partial}{\partial x_i}\left(\rho\, u_i\, h\right) \quad = \quad \frac{\partial p}{\partial t}+u_i\frac{\partial p}{\partial x_i}-\frac{\partial j_i^q}{\partial x_i}+\tau_{ij}\frac{\partial u_i}{\partial x_j}+\dot{Q}\,. \tag{2.31}$$

Since h considers the enthalpy of formation (Eq. 2.13, Eq. 2.14), Equation 2.31 does not include a chemical source term. The transient pressure term can be neglected in open flames but is important in IC engines, where pressure changes significantly in time. The convective change of pressure does not need to be considered if one is interested in the small Mach number limit only. According to Hirschfelder et al. [45], the heat flux j_i^q can be decomposed as follows

$$j_i^q \quad = \quad j_i^{qc}+j_i^{qd}+j_i^{qD}\,. \tag{2.32}$$

j_i^{qc} accounts for heat diffusion and can be expressed by *Fourier's law* according to

$$j_i^{qc} \quad = \quad -\lambda\frac{\partial T}{\partial x_i}\,, \tag{2.33}$$

where λ denotes the thermal conductivity. j_i^{qd} is the heat flux due to mass diffusion of species with different levels of enthalpy, and it is relevant for multicomponent gases only. It is defined by

$$j_i^{qd} \quad = \quad \sum_{k=1}^{N} h_k\, j_{ki}\,. \tag{2.34}$$

j_i^{qD} is associated with the *Dufour-effect*. It accounts for the heat flux due to species mass fraction gradients. It can be interpreted as the reciprocal phenomenon to the *Soret-effect*. The Dufour-effect is usually neglected in combustion processes (Hirschfelder et al. [45]). Differentiating Equation 2.14 one obtains

$$\mathrm{d}h = c_p\mathrm{d}T+\sum_{k=1}^{N} h_k\mathrm{d}Y_k\,. \tag{2.35}$$

By combining Equations 2.35, 2.34, 2.33, and 2.28, the heat flux takes the form

$$j_i^q = -\frac{\lambda}{c_p}\frac{\partial h}{\partial x_i}+\sum_{k=1}^{N} h_k\left(\frac{\lambda}{c_p}-\frac{\mu}{Sc_k}\right)\frac{\partial Y_k}{\partial x_i}\,. \tag{2.36}$$

Now, by introducing the Prandtl number

$$Pr = \frac{\mu c_p}{\lambda}, \tag{2.37}$$

which compares molecular momentum and heat transport, it follows that

$$j_i^q = -\frac{\mu}{Pr}\frac{\partial h}{\partial x_i} + \sum_{k=1}^{N} h_k \left(\frac{\mu}{Pr} - \frac{\mu}{Sc_k}\right)\frac{\partial Y_k}{\partial x_i}. \tag{2.38}$$

In order to simplify Equation 2.38, it is assumed that the Lewis number $Le_k = Sc_k/Pr$ equals unity. This constitutes a situation where mass and heat diffuse in the same way and no differential diffusion occurs. Hence, Equation 2.38 can be written as

$$j_i^q = -\frac{\mu}{Pr}\frac{\partial h}{\partial x_i}. \tag{2.39}$$

The last term $\dot{Q}$ in Equation 2.31 represents a heat source term due to e.g. a spark plug or wall heat transfer.

2.2 PHENOMENOLOGICAL DESCRIPTION OF TURBULENCE

2.2.1 *Scales of Turbulent Motion*

The term *scales* is used in a great variety of contexts and meanings in the description of turbulent flows. For example, it is frequently used in physical space and in Fourier space without much distinction. This ambiguity of language is one (among others) of the main difficulties of the inherent problems in turbulence theories. Another difficulty is that different scales are not as separated as usually assumed. Hence, the distinction between large and small scales is quite problematic, though useful from the technical point (Tsinober [117]). There are several useful scales that are statistically defined quantities and not some specific physical scales. The most prominent scales are those defined by Kolomogorov. According to the first similarity hypothesis of Kolmogorov, the energy in the viscous subrange is uniquely determined by the fluid kinematic viscosity ν and the turbulent dissipation rate ϵ in case of high Reynolds numbers. Due to viscosity effects, the energy dissipates at the smallest turbulent scales according to the turbulent dissipation rate. Hence, the length scale of these eddies must be a function of these two quantities only. Based on dimensional analysis, the Kolmogorov length scale η can be defined as

$$\eta = \left(\frac{\nu^3}{\epsilon}\right)^{\frac{1}{4}}. \tag{2.40}$$

This length scale is considered as the smallest spatial scale in turbulence. Similarly, the corresponding time and velocity scales are defined as

$$t_\eta = \sqrt{\frac{\nu}{\epsilon}} \quad \text{and} \quad u_\eta = (\nu\epsilon)^{\frac{1}{4}}. \tag{2.41}$$

It is known that adequate resolution in space and time in laboratory and numerical experiments is achieved if the smallest resolved scales are of the order of the Kolmogorov scales.

By assuming scale-invariance of ϵ, the energy dissipation rate can also be used to derive the turbulent length scale

$$l_t = \frac{k^{\frac{3}{2}}}{\epsilon}\,, \tag{2.42}$$

which is associated with the size of the larger integral eddies. The turbulent kinetic energy k is defined as half of the trace of the Reynolds-stress tensor

$$k = \frac{1}{2}\overline{u_k' u_k'}\,. \tag{2.43}$$

The time scale that is associated with the most energetic eddies is referred to as the integral time scale τ with

$$\tau = \frac{k}{\epsilon}\,. \tag{2.44}$$

The root-mean-square (RMS) of the velocity fluctuations, u'_{RMS}, is related to the turbulent kinetic energy by

$$u'_{RMS} = u' = \sqrt{\frac{2}{3}k}\,. \tag{2.45}$$

In the literature, u'_{RMS} is often referred to as turbulence intensity denoted by u' or v', respectively. It has to be noted that Equation 2.45 is strictly valid only for isotropic turbulence. The relation between the characteristic scales can be obtained by introducing the turbulent Reynolds number

$$Re_t = \frac{u' l_t}{\nu}\,. \tag{2.46}$$

This leads to the following correlations between the Kolmogorov and integral scales

$$\frac{\eta}{l_t} = (Re_t)^{-3/4}\,, \quad \frac{t_\eta}{\tau} = (Re_t)^{-1/2}\,, \quad \frac{u_\eta}{u'} = (Re_t)^{-1/4}\,. \tag{2.47}$$

The integral scales are in some sense the largest relevant scales of the system. Turbulent fluctuations in regions separated by scales much larger than the integral ones both in space and time do not influence each other. The two-point velocity correlation R_{ij} relates the velocity fluctuations of two points with distance $r = |\mathbf{r}|$ and indicates to what degree they influence each other

$$R_{ij}(\mathbf{r},\mathbf{x},t) = \overline{u_i'(\mathbf{x},t)u_j'(\mathbf{x}+\mathbf{r},t)}\,. \tag{2.48}$$

For $|\mathbf{r}| = 0$ the Reynolds-stress tensor is recovered. Based on the two-point correlation, various length scales such as the integral length scale L_{ij}^k can be defined according to

$$L_{ij}^k = \frac{1}{R_{ij}(0,\mathbf{x},t)}\int_0^\infty R_{ij}(r_k,\mathbf{x},t)\,\mathrm{d}r_k\,. \tag{2.49}$$

If the velocity vectors at the two locations and the distance vector point in the same direction, the length scale is referred to as the longitudinal integral length scale

$$L_{11}^1 = \frac{1}{\overline{u_1'^2}}\int_0^\infty R_{11}(r_1,\mathbf{x},t)\,\mathrm{d}r_1\,. \tag{2.50}$$

Similar to l_t, L_{11}^1 is associated to the large energy-containing eddies. Pope [93] has shown that in the limit of high Reynolds numbers the ratio L_{11}^1/l_t tends asymptotically to a value of 0.43. The Taylor micro length scale, l_λ, is defined from the relation

$$l_\lambda = \left(\frac{\overline{u_1'^2}}{\partial^2 R_{11}/\partial r_1^2}\right)^{1/2}\,. \tag{2.51}$$

In the limit of high Reynolds numbers it can be shown that l_λ is intermediate in size between the integral length scale l_t and the Kolomogorov scale η. The Taylor scale does not have a clear physical interpretation (Pope [93]). However, it is used in some turbulence theories to define the Taylor-scale Reynolds number

$$R_\lambda = \frac{u' l_\lambda}{\nu}\,. \tag{2.52}$$

For a more detailed description of the various important length scales the reader is referred to Rotta [100] and Pope [93].

2.2.2 *The Statistical Description of Turbulence*

In turbulent flows, the instantaneous realization of the velocity components and scalars such as mass fractions and temperature are stochastic, fluctuating quantities. It is, therefore, convenient to describe and to characterize the stochastic nature of these variables by using the probability theory. In the following, various probability functions are defined and outlined in order to provide a theoretical foundation of the statistical approach. A more comprehensive review of statistical methods for turbulent flows is given by Pope [91], Pope [93], and Klimenko and Bilger [52].

The instantaneous realization of a velocity component $u(\mathbf{x}, t)$ at a specific point in space and time in a turbulent flow can be considered as a random variable. The aim of the statistical approach is to determine the probabilities of u instead of trying to predict the instantaneous value, since this value is indeterminable. The probability p of finding a value of $u < U$ is defined by the cumulative distribution function (CDF) $F_u(U)$ given by

$$F_u(U) = p\{u < U\}\,, \tag{2.53}$$

where the independent scalar variable U is referred to as the sample space variable corresponding to u. The significance of the sample space variable U is that it consists of all possible realizations of the random variable u. Since every event of u can be associated with a region in sample space, the probability of the event is equal to the region in sample space. Thus, the probability of the event $U_a \leq u < U_b$ can be defined as

$$p\{U_a \leq u < U_b\} = F_u(U_b) - F_u(U_a)\,. \tag{2.54}$$

The probability density function (PDF) $P_u(U)$ of the random variable u is the derivative of the distribution function $F_u(U)$

$$P_u(U) = \frac{\mathrm{d}F_u(U)}{\mathrm{d}U}\,. \tag{2.55}$$

It follows that the probability of u in a given interval is equal to the integral of the PDF over the corresponding region in sample space

$$\int_{U_a}^{U_b} P_u(U)\,\mathrm{d}U = F_u(U_b) - F_u(U_a)\,. \tag{2.56}$$

For an infinitesimal region it follows

$$P_u(U)\mathrm{d}U = p\{U \leq u < U + \mathrm{d}U\}\,. \tag{2.57}$$

Since F_u is a non-decreasing function of u, its derivative $P_u(U)$ cannot be negative

$$P_u(U) \geq 0\,. \tag{2.58}$$

Another fundamental property of the probability function is that it satisfies the normalization condition

$$\int_{-\infty}^{+\infty} P_u(U)\,\mathrm{d}U = 1\,, \tag{2.59}$$

which simply states that the probability of the event $-\infty \leq u < +\infty$ is certain. Once the PDF of a variable is known, one may define its moments defined by

$$\overline{u^n} = \int_{-\infty}^{+\infty} U^n P_u(U)\,\mathrm{d}U\,, \tag{2.60}$$

where the overbar denotes the average or expectation of u^n. The central moments are defined according to

$$\overline{[u-\overline{u}]^n} = \int_{-\infty}^{+\infty} (U-\overline{u})^n P_u(U)\,\mathrm{d}U\,. \tag{2.61}$$

The mean $\overline{u}$ of the random variable u corresponds to the first moment $(n = 1)$ and defines the center of the PDF, in that the first central moment of u is zero $(\overline{u - \overline{u}} = 0)$. In general, let $g(u)$ be a function of the random variable u, then the mean of g is defined as

$$\overline{g} = \int_{-\infty}^{+\infty} g(U) P_u(U)\,\mathrm{d}U\,. \tag{2.62}$$

The fluctuation of u, u', is defined as the deviation from the mean $\overline{u}$. Thus, the instantaneous realization of the velocity component can be split into its mean and its fluctuation

$$u = \overline{u} + u'\,. \tag{2.63}$$

The variance $\overline{u'^2}$ is the mean of the square of the fluctuation

$$\overline{u'^2} = \overline{(u-\overline{u})^2}\,, \tag{2.64}$$

and is referred to as the second central moment

$$\overline{[u-\overline{u}]^2} = \int_{-\infty}^{+\infty} (U-\overline{u})^2 P_u(U)\,\mathrm{d}U\,. \tag{2.65}$$

The square root of the variance, $\sqrt{\overline{u'^2}}$, defines the standard deviation and is a measure of the width of the probability density function.

Up to this point, only single random variables have been considered. In case of the three-dimensional Navier-Stokes equations, the velocity components and the pressure depend on each other and are correlated. Hence, it is not sufficient to determine the distribution function for each variable separately, since they do not contain information of the joint (simultaneous) event. This information is provided by the joint distribution function. In the following, the properties of the joint PDF are discussed by introducing the joint distribution function F_{uv} of the velocity components u and v

$$F_{uv} = p\{u < U, v < V\}\,, \tag{2.66}$$

where U and V are the sample space variables of the velocity components. The joint PDF of U and V, $P_{uv}(U,V)$, is defined by

$$P_{uv}(U,V) = \frac{\partial^2 F_{uv}}{\partial U \partial V}\,. \tag{2.67}$$