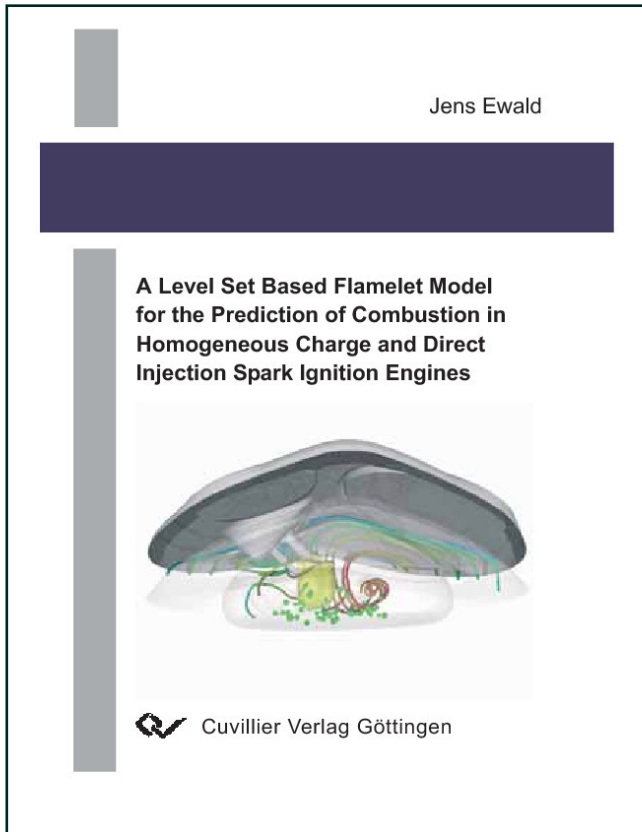




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A Level Set Based Flamelet Model for the Prediction of Combustion in Homogeneous Charge and Direct Injection Spark Ignition Engines



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Chapter 1

Introduction

Combustion has been one of mankind's oldest technologies to convert chemical energy into heat or mechanical energy. Although there have been many attempts to supersede that technology, for example by fuel cells, photovoltaics, not to mention nuclear technology, it seems likely that in the near and intermediate future combustion will still play an important role for the exploitation of energy sources, provided either by means of fossil fuels or by other, renewable energy sources. Today, growing global demand for individual means of transportation, increasing implications on environmental issues, and future possible penury of fossil fuels make it even more important to intensify the efforts in improving existing energy conversion technologies. With respect to passenger cars, for example, internal combustion engines will still play a viable role in those efforts. Here, two major important research directions can be identified; these are High-Pressure Direct Injection Diesel engines (f. ex. Common-Rail based systems) and Direct Injection Spark Ignition (DISI) gasoline engines.

Unfortunately, the development of new strategies for internal combustion engines today is increasingly costly for additional gain in fuel efficiency and further reduction of pollutant emissions. In order to reduce development costs and enhance the number of parameters studied to optimize, the concept of Computational Fluid Dynamics (CFD) is becoming more and more important. Internal Combustion engines are subjected to the combined physics of chemistry, fluid mechanics and turbulence theory. Even though the microscopic interaction between these three topics is probably sufficiently understood, prediction of problems pertinent to industrial scale applications using Direct Numerical Simulation (DNS) of these mechanisms is not possible at present and will remain impracticable in the foreseeable future.

This dilemma necessitates the development of physical sub-models for turbulent flows and combustion on a macroscopic scale. These models do not only enable the numerical simulation of engineering applications with combustion. Also the macroscopic physical mechanisms of flow, turbulence, and combustion can be understood by researchers and engineers and thus may lead to additional approaches for technology

improvement.

This work focuses on the further development of turbulent premixed combustion modeling which is the main mechanism of combustion in DISI gasoline engines. The goal of this model is to understand the influence parameters on turbulent flame propagation in the engine and finally the kinematics of the turbulent flame front. Employing this information, global data as the heat release and the pressure trace can be predicted. It is possible to visualize where and when combustion in the chamber occurs. Coupled with a corresponding prediction model, eventually pollutant production could be calculated.

For most of (DI)SI engine operation modes it can be assumed that turbulent premixed combustion takes place in the so-called *flamelet regime*. This regime is furnished with a complex fractal-like distribution of laminar premixed flame structures that are surrounded by turbulent eddies of an otherwise non-reacting flow. The microscopic complexity of the combined physics addressed above can in this case be simplified by model assumptions since the time and length scales of the turbulent flow on the one hand and the chemistry of the laminar flame on the other hand are decoupled up to a certain order of magnitude.

With regards to premixed turbulent combustion modeling two major approaches exist which describe the structure of the turbulent premixed flame front. The first approach is called *progress variable approach* in which modeling is based on the local mean premixed reaction rate formulation for a burnt gas mass fraction transport equation. While models based on this equation type can easily be implemented into existing CFD computer programs since the methodology essentially follows the one for reactive species, difficulties arise in regions where the premixed flame front is very thin compared to the numerical grid used for the computation. This is also an attribute for the transition from laminar to turbulent flames.

The other approach is based on *Level Sets* which was first derived for laminar flame configuration initially by *Williams* [110]. Those Level Sets describe the flame front as a surface for which a kinematic equation can be postulated. This approach was extended by *Peters* [69, 68] into the turbulent regime by introducing a second model equation for the turbulent flame brush thickness. Due to the kinematic approach, the modeling is based on the formulation of a turbulent burning velocity instead of a local reaction rate. This model is able to give a consistent representation of a premixed flame in the laminar as well as in the turbulent regime. It was chosen to be the basis in this work although the implementation into a CFD code requires additional efforts. Due to the nature of the equation to be solved a different numerical solver other than one for conserved and reactive scalars needs to be employed. In most CFD codes, also initially in the code AC-FluX used in this work, an appropriate solver is not per se implemented.

In this work, a further development of the original combustion model by *Peters* [70, 71] is presented. The original model was developed and validated on averaged stationary turbulent flames, that is fully premixed [42] and partially premixed flames [13]. This model then was extended by the author in order to also consistently predict premixed flame propagation during the stage of turbulent flame development in which

the original model still is a sub-set of the new model. In order to predict the dynamics of spark ignition the new model was then formulated for a spherical flame kernel. In contrast to other approaches [99] the model developed in this work employs the same model for the phase of the spark ignition as well as for the later stages of turbulent flame development and flame propagation. Additionally, flame-wall interactions and effects of mean flame front curvature are studied.

This work is structured as follows: In chapter 2 the basic physical principles of fluid dynamics and turbulent flows are discussed. With respect to the turbulence modeling, a statistical approach towards Reynolds Averaged Navier-Stokes equations (RANS) is presented. Starting from this review, in the following chapter 3 the theory of turbulent premixed flow is derived. This chapter is subdivided into a discussion of the physics of turbulent flows, and modeling of turbulent flame propagation based on progress variable and Level Set approaches. Chapter 4 presents the numerical implementation of the G -equation model into the research code that was used for the validations in chapter 5. The validation is performed at first on a simple combustion setup in a cylindrical vessel carried out by *Hamamoto et al.* [36]. Following from there, numerical results employing the G -equation model are compared against experimental results obtained from a DISI spray guided gasoline engine. This engine was operated for this comparison in homogeneous charge as well as in stratified charge mode. This work closes with conclusions and an outlook to future research in chapter 6. In the appendix, also the numerical method in order to solve numerically for the Level Set transport equation is explained and an approximative expression for the determination of the laminar burning velocity of rich and lean iso-octane/air mixtures including Exhaust Gas Recirculation (EGR) is presented.

Chapter 2

Physics of Fluid Dynamics

In this chapter we will discuss the fundamental principles of Fluid Dynamics and turbulent flows as they are needed in this work. The first section deals with the fundamental equations as they can directly be derived from kinetic gas theory. This appears as overly extensive to be presented in this framework because the equations will not be used in that form. However, the simplifications that already on this level of modeling are applied need to be pointed out. This presentation includes basic principles of elementary reaction kinetics and the introduction of mixture states descriptors such as the mixture fraction Z . Continuing from there, basic principles of turbulent flows are briefly discussed. This includes an introduction of statistical principles as well as the description of conventional and Favre averaging. At last, the Reynolds Averaged Navier Stokes turbulence modeling approach is presented.

2.1 Fundamental Equations of Fluid Dynamics

The fundamental transport equations of Fluid Dynamics are based on the so-called Navier-Stokes equations. The Navier-Stokes equations can be derived by a heuristic approach, that is, the governing differential equations are in this case derived by assuming space continuity and applying macroscopically observable quantities like pressure, density, tension, mass flux, etc. to infinitesimally small control volumes.

Based on kinetic gas theory, a mathematically more rigorous ansatz (i.e. an ad-hoc assumption) can be followed as well. This mathematical approach is based on statistical mechanics and the kinetic theory of gas dynamics. A comprehensive treatment of this topic can be found in pertinent monographs, f. ex. *Ferziger et al.* [27], *Chapman and Cowling* [12], and *Giovangigli* [31]. While the first two references focus on the physics of kinetic transport by gas diffusion, the last reference emphasizes the numerical issues of solving the equations for determining the diffusion velocities and coefficients. In the following, the fundamentals of this theory will only briefly be discussed and finally the resulting Navier-Stokes equations will be given.

The kinetic theory parametrizes the gas molecules as particles propagating in a multi-dimensional parameter space. For monoatomic molecules, only six dimensions are necessary, these are the molecule position \vec{r} and the molecule velocity \vec{c} . For polyatomic molecules, additional dimensions are required which describe the rotational state of the molecules.

The further derivations are based on mainly two assumptions:

- The gas density is low. As a consequence only pairs of particles do interact with each other. This requirement is fulfilled for the problems treated in this work.
- The validity of the so-called ‘‘Stoßzahlansatz’’ as postulated by Boltzmann [6]. This approach assumes non-deterministic particle propagation and molecular chaos thus leading to an irreversibility of particle interaction events.

As a result the so-called Boltzmann-equations can be derived. Core of these equations is the velocity distribution function f . The macroscopic quantities density ρ , velocity \vec{u} , and pressure p can be expressed as different integral moments of f .

In order to yield the macroscopic conservation equations, the so called Chapman-Enskog method asymptotically expands the differential equation f into a series of powers of a small expansion parameter. Based on the assumption of a state near to thermodynamical equilibrium, the Boltzmann equations are thus linearized. Using such an expansion approach for f , the transport equations can be derived employing the linearized Boltzmann equations. An approximation of zero order yields the Euler equations of gas dynamics. Using a first order approximation of f , the Navier-Stokes equations are obtained. Those comprise the Euler equations extended by transport terms due to molecular viscosity and diffusivity. Then, the resulting transport equations for the velocity, the enthalpy h , and the species mass fractions Y_α for species α read:

$$\frac{\partial \rho \vec{u}}{\partial t} + \nabla \cdot (\rho \vec{u} \circ \vec{u} + p \bar{I}) = -\nabla \cdot \bar{\Pi} + \sum_{\alpha} \rho b_{\alpha}^{\vec{}} \quad (2.1)$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho h \vec{u}) = -\nabla \cdot \vec{Q} - \bar{\Pi} : \nabla \circ \vec{u} + \sum_{\alpha} \vec{F}_{\alpha} \cdot b_{\alpha}^{\vec{}} + \frac{\partial p}{\partial t} + \vec{u} \cdot \nabla p \quad (2.2)$$

$$\frac{\partial \rho Y_{\alpha}}{\partial t} + \nabla \cdot (\rho Y_{\alpha} \vec{u}) = -\nabla \cdot \vec{F}_{\alpha} + W_{\alpha} \dot{\omega}_{\alpha} . \quad (2.3)$$

Before we focus on the definition of the the viscous tensor $\bar{\Pi}$ we will introduce the rate-of-strain tensor \bar{S}^*

$$\bar{S}^* = S_{ij}^* = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \quad (2.4)$$

and the rate-of-rotation tensor

$$\bar{\Omega} = \Omega_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right) , \quad (2.5)$$

decomposing the velocity gradient tensor $\partial u_i/\partial x_j$ into a symmetric and an anti-symmetric component. Here, however, we will employ a modified definition for the rate-of-strain tensor eqn. (2.4),

$$\bar{\bar{S}} = S_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{1}{3} \frac{\partial u_l}{\partial x_l} \delta_{ij} , \quad (2.6)$$

in which for compressible flows the strain tensor is made traceless. Then, the viscous tensor $\bar{\bar{\Pi}}$ is defined using the volume viscosity κ and the shear viscosity η as

$$\bar{\bar{\Pi}} = -\kappa(\nabla \cdot \vec{u})\bar{\bar{I}} - \eta 2\bar{\bar{S}} . \quad (2.7)$$

The equation for the enthalpy (2.2) does not contain a source term due to chemical reactions since h is the total enthalpy which includes the chemical heat of formation. The acceleration vector \vec{b}_α indicates external forces (e.g. gravity).

For the conservation equations of enthalpy and species α , an expression for the species mass fluxes

$$\vec{F}_\alpha = -\rho Y_\alpha \vec{V}_\alpha \quad (2.8)$$

is needed, which is based on the species diffusion velocities

$$\vec{V}_\alpha = - \sum_{\beta} D_{\alpha\beta} (\vec{d}_\beta + \chi_\beta \nabla \log T) \quad (2.9)$$

with the multicomponent diffusion coefficients $D_{\alpha\beta}$ of species α into species β and the thermal diffusion ratio χ_β . The diffusion driving forces \vec{d}_α do not only comprise the effects of species concentration gradients and external forces but also the pressure gradient:

$$\vec{d}_\alpha = \nabla \left(\frac{p_\alpha}{p} \right) + \left(\frac{p_\alpha}{p} - \frac{\rho_\alpha}{\rho} \right) \nabla \log p + \frac{\rho_\alpha}{p} \left(\frac{\sum_{\beta} \rho_\beta \vec{b}_\beta}{\rho} - \vec{b}_\alpha \right) . \quad (2.10)$$

The species concentrations are expressed in this equation as the ratios of the density ρ_α and partial pressure p_α to the total density ρ and pressure p , respectively. The heat flux vector \vec{Q} is based on the expressions given above and the thermal conductivity λ ,

$$\vec{Q} = \sum_{\alpha} h_\alpha \vec{F}_\alpha - \lambda \nabla T + p \sum_{\alpha} \chi_\alpha \vec{V}_\alpha . \quad (2.11)$$

In many problems, these fundamental equations are simplified for analysis. This applies mainly to the determination of the diffusion fluxes. Here, we will neglect effects of thermal diffusion $\chi_\beta D_{\alpha\beta}$ and diffusion due to pressure gradients. Additionally, instead of multicomponent diffusion coefficients, mean diffusivities $D_{\alpha\beta} \approx D_\alpha$ for each species are assumed.

Summing up eqns. (2.3) over all species k ,

$$\rho = \sum_{\alpha} \rho_{\alpha} = \sum_{\alpha} \rho Y_{\alpha} \quad (2.12)$$

the continuity equation is obtained.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0 \quad (2.13)$$

The only terms of the eqns. (2.3) that still need to be closed are the chemical reaction rates $\dot{\omega}_{\alpha}$. Each of the reaction rates contains the rates of progress τ_t of any elementary reactions r multiplied by the stoichiometric coefficients ν of species α in reaction r

$$\dot{\omega}_{\alpha} = \sum_r \nu_{\alpha r} \tau_r = \sum_r (\nu_{\alpha r}^b - \nu_{\alpha r}^f) \tau_r . \quad (2.14)$$

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

$$\tau_r = K_r^f \prod_{\beta} [X]_{\beta}^{\nu_{\alpha\beta}^f} - K_r^b \prod_{\beta} [X]_{\beta}^{\nu_{\alpha\beta}^b} . \quad (2.15)$$

For the forward rate constants usually an approach similar to the generalized Arrhenius empirical relation

$$K_r^f = A_r T^{n_r} \exp\left(-\frac{E_r}{R_m T}\right) \quad (2.16)$$

is employed. Here A_r is the frequency factor of the reaction, R_m the gas constant, E_r the activation energy of the reaction, and n_r a non-dimensional exponent. The relation (2.16) can then also be employed for the backward rate constant, but in most cases K_r^b is linked with K_r^f by an equilibrium constant $K_{c,r}$ (for further information one may refer to standard literature, e.g. [29]):

$$K_{c,r} = \frac{K_r^f}{K_r^b} . \quad (2.17)$$

2.1.1 Equation of state

For the link between temperature, species distribution, density, and pressure, the ideal gas law is employed. With the ideal gas constant \mathcal{R} the relationship reads:

$$\frac{p}{\rho} = \sum_{\alpha} \frac{Y_{\alpha}}{W_{\alpha}} \mathcal{R} T . \quad (2.18)$$