

### Stefan Emil Vogel (Autor) Simulation of Lifted Diesel Sprays Using a Combined Level-Set Flamelet Model



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# **1** Introduction

A common goal for numerical combustion simulation is to be able to explain, improve, and set guidelines for the combustion in gas turbines, technical processes, and for all types of internal combustion engines. Improving the current engines means that the pollutants need to be reduced without loosing, or even gaining, efficiency of the combustion process. Since it is impossible to describe the turbulent combustion in very detailed resolution in an acceptable amount of time, models are used which need to be extended in order to improve their capability to predict newly developed and still undefined operating conditions.

Diesel engines are successfully used for various applications, for example in power generation and passenger cars. One advantage of the Diesel engine is the low fuel consumption and high efficiency, respectivly. Currently, more than 50% of the newly registered cars are equipped with a Diesel engine. Therefore, it is very important to decrease the emissions, especially soot and  $NO_x$ . Several new Diesel combustion concepts have been proposed and tested in combustion vessels. One of these concepts is the usage of lifted Diesel flames.

Pickett et al. [62, 63] observed that for very small Diesel sprays no detectable amount of soot is formed inside the flame. The reason for this effect is the spatial separation of the fuel-rich zones from the combustion; therefore, more time is available to premix oxidizer and fuel. This results in a leaner and more premixed-like combustion, where less soot precursors are formed. For this kind of combustion mode, the resulting lift-off length (LOL) has to be larger than the liquid penetration length of the fuel. Otherwise, rich pockets would be formed out of evaporation in already existing burning



Figure 1.1: Example of a high-sooting (left) and low-sooting (right) lifted Diesel flame

zones, which would not be able to burn in a lean premixed mode like the previously evaporated gaseous fuel mass. A very high LOL is desired to reach the effect of low or non-sooting conditions. An example of two different lifted Diesel flames is depicted in Fig. 1.1.

The first step is to understand the underlying physics of the lift-off phenomenon under Diesel-engine like conditions. But it is still doubtful and being discussed in the combustion community which physical process is accountable for the stabilization of the flame. This work provides new information and explanations on the underlying physics of the lift-off process.

A major focus of this work is to extend the flamelet model for non-premixed combustion to be able to also calculate premixed and partially premixed combustion. The result is a model which incorporates flame propagation and prediction of multiple auto-ignition spots. The commonly used Representative Interactive Flamelet (RIF) concept [4–6, 26–28, 67, 70] is first extended to the Multiple-injected Representative Interactive Flamelet (MRIF) model, which is close to the one used by Barths [3]. A similar approach was recently developed by Magnusson [39]. Upon MRIF, the combustion model G-equation coupled with MRIF (G-MRIF) is developed, which additionally includes the ability to describe a turbulent premixed flame propagation using the G-equation model [16, 60]. This new combustion model is applied to different lifted Diesel-combustion conditions to provide information on the performance and predictability of the G-MRIF model. Furthermore, the acquired knowledge is used to discuss the possible phenomena of the LOL.

# 2 Description of the flow field

The solution of the turbulent flow field is necessary as an input for the modeling of heat release and pollutant formation for all detailed combustion models. In this chapter, the basic equations are described and discussed, which are used in the Advanced Combustion Flux-Solver (AC-FluX) flow and chemistry solver. Later in this thesis different combustion models for premixed and non-premixed combustion are introduced. Finally, the coupling of the extended flamelet model for non-premixed (MRIF) and the premixed flamelet model (G-equation) into the G-MRIF model are discussed.

## 2.1 Flow-field equations

To be able to describe the flow field of the gaseous phase, coupled partial differential equations for the continuity (2.1), momentum (2.2), and enthalpy (2.4) have to be solved.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_{\alpha}} \left( \rho v_{\alpha} \right) = \rho \dot{S} , \quad \alpha = 1, 2, 3$$
(2.1)

 $\dot{S}$  is the mass source through evaporation of liquid parcels. The following equation is solved for the conservation of the momentum:

$$\frac{\partial}{\partial t}\left(\rho v_{\alpha}\right) + \frac{\partial}{\partial x_{\beta}}\left(\rho v_{\alpha} v_{\beta}\right) = -\frac{\partial p}{\partial x_{\alpha}} + \frac{\partial \tau_{\alpha\beta}}{\partial x_{\beta}} + f_{\alpha}^{s}, \quad \alpha = 1, 2, 3.$$
(2.2)

Coupling between the gaseous phase and the liquid phase is based on the source term  $f^s_{\alpha}$ . For a Newtonian fluid a symmetrical stress tensor  $\tau_{\alpha\beta}$  according to equation (2.3) can be assumed.

$$\tau_{\alpha\beta} = \rho\nu \left(\frac{\partial v_{\alpha}}{\partial x_{\beta}} + \frac{\partial v_{\beta}}{\partial x_{\alpha}}\right) - \frac{2}{3}\rho\nu \frac{\partial v_{\gamma}}{\partial x_{\gamma}}\delta_{\alpha\beta}$$
(2.3)

The energy conservation is defined according to the following equation:

$$\frac{\partial}{\partial t}\left(\rho h\right) + \frac{\partial}{\partial x_{\alpha}}\left(\rho v_{\alpha} h\right) = \frac{\partial p}{\partial t} + v_{\alpha} \frac{\partial p}{\partial x_{\alpha}} - \frac{\partial j_{\alpha}^{q}}{\partial x_{\alpha}} + \dot{q}_{s} , \qquad (2.4)$$

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in which  $\rho$  is the density,  $v_{\alpha}$  the velocity,  $\dot{q}_s$  the source term, h the enthalpy, and p the pressure. For compressible flows the equations are closed using equations of state (2.5 - 2.7).

$$\frac{p}{\rho} = R_{\rm gas} \sum_{i=1}^{n_s} \frac{Y_i}{M_i} T \tag{2.5}$$

$$h_{i} = \Delta h_{f,i}^{0} + \int_{T^{0}}^{T} c_{p_{i}} \, \mathrm{d} T$$
(2.6)

$$h = \sum_{i=1}^{n_s} Y_i h_i \tag{2.7}$$

In equations (2.5 - 2.7) all single species are summed over all species  $n_s$ , which is the number of species the gaseous phase is based on. The single enthalpy  $h_i$  is calculated using a reference value  $h_{f,i}^0$  and the heat capacity at constant pressure  $c_{p_i}$  for the species i.  $R_{gas}$  denotes the universal gas constant and  $M_i$  the molar mass of the species.  $Y_i$  describes the species mass fraction of the species i.

The heat flux vector  $j_{\alpha}^{q}$  is defined by thermal diffusion and by the enthalpy transport through molecular diffusion, according to:

$$j_{\alpha}^{q} = -\lambda \frac{\partial T}{\partial x_{\alpha}} + \sum_{i=1}^{n_{s}} j_{i,\alpha} h_{i} .$$

$$(2.8)$$

Additionally, the mass fractions of the species are conserved (2.9). The first term on the left side describes the local change and the second the convective transport. On the right, the first term describes the molecular diffusion, which is defined using equation (2.10), and the second term describes the chemical source term.

 $v_{i,\alpha}$  in equation (2.10) is the velocity of the chemical species *i* and  $j_{i,\alpha}$  the resulting mass flow of the species *i*.

$$\frac{\partial}{\partial t} \left( \rho Y_i \right) + \frac{\partial}{\partial x_\alpha} \left( \rho v_\alpha Y_i \right) = \frac{\partial j_{i,\alpha}}{\partial x_\alpha} + \rho \dot{S}_{Y_i} \tag{2.9}$$

$$j_{i,\alpha} = \rho(v_{i,\alpha} - v_{\alpha}) \tag{2.10}$$

 $j_{i,\alpha}$  can also be described using the Fick's first law (2.11), where  $D_i$  is denoted as the diffusion coefficient of species *i*.

$$j_{i,\alpha} = -\rho D_i \frac{\partial Y_i}{\partial x_\alpha} \tag{2.11}$$

Applying the first Fick's law (2.11) leads to:

$$\frac{\partial}{\partial t} \left( \rho Y_i \right) + \frac{\partial}{\partial x_\alpha} \left( \rho v_\alpha Y_i \right) = \frac{\partial}{\partial x_\alpha} \left( \rho D_i \frac{\partial Y_i}{\partial x_\alpha} \right) + \rho \dot{S}_{Y_i} . \tag{2.12}$$

#### **Chemical Source Terms**

Chemical source terms are based on equation (2.13):

$$\dot{m}_i = M_i \sum_{ir=1}^{n_r} (\nu_{i,ir}'' - \nu_{i,ir}') k_{ir} \prod_{j=1}^{n_s} c_j^{\nu_{j,ir}'}$$
(2.13)

 $M_i$  denotes the molar mass of the species i,  $n_r$  is the number of elementary reactions,  $\nu'_{i,ir}$  and  $\nu''_{i,ir}$  are the stoichiometric coefficients of the species i in the reactions ir, and  $c_j$  is the concentration of the species j. The reaction rate  $k_{ir}$  is given through the Arrhenius formulation:

$$k_{ir} = A_{ir} T^{n_{ir}} \exp\left[-\frac{E_{ir}}{R_{gas}T}\right].$$
(2.14)

The frequency factor  $A_{ir}$ , exponent  $n_{ir}$ , and activation energy  $E_{ir}$  are defined by the corresponding reaction mechanism.

#### Heat loss through radiation

Heat loss through radiation is based on two physical effects:

- gas radiation
- soot radiation

Kirchhoff's emission law for gray emitters with  $\epsilon$  as the emission coefficient leads to:

$$\dot{q}_r = 4\epsilon \alpha_p \sigma_s T^4 \,. \tag{2.15}$$

 $\sigma_s = 5.669 * 10^{-8} \text{ W/(m^2 K^5)}$  is the Stefan-Boltzmann constant and  $\alpha_p$  Planck's radiation coefficient, according to Eq. (2.16).

$$\alpha_p = \alpha_{p,s} f_v + \alpha_{p,CO_2} p_{CO_2} + \alpha_{p,H_2O} p_{H_2O}$$
(2.16)

 $f_v$  is the soot volume fraction. The remaining coefficients  $\alpha_{p,CO_2}$  and  $\alpha_{p,H_2O}$  are taken from Müller [42], which leads to:

$$\dot{q}_r = 4\epsilon \sigma_s T^4 (\alpha_{p,s} f_v + \alpha_{p,CO_2} p_{CO_2} + \alpha_{p,H_2O} p_{H_2O}).$$
(2.17)

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# 2.2 Description of the turbulent flow and mixing field

Nearly all technical applications of combustion are turbulent. Turbulence occurs when a critical Reynolds-number is reached and the viscosity is not able to damp out instabilities of the flow. The flow gets turbulent and larger turbulent eddies are generated, which finally cause smaller eddies. The kinetic energy of the mean flow transfers parts of its energy into big turbulent structures. These structures transport the energy by an *energy cascade* into smaller turbulent structures [37]. Finally, the kinetic energy gets dissipated in the smallest eddies by the laminar viscosity. It should also be mentioned that turbulence is not just influencing the momentum exchange of the flow ("turbulent viscosity"), but also improves the mixing process tremendously [23, 34, 60].

### 2.2.1 Scales of turbulent flows

Since the energy is dissipated at the smallest scales, which was already proposed by Kolmogorov [34], the energy has to originate from the bigger eddies. Opposed to the big eddies, the smallest eddies are assumed to be isotropic and therefore have a universal character. According to Pope [71], the turbulent length scales can roughly be subdivided into two sections:

- energy-containing range
- universal equilibrium range, with suranges given by
  - inertial range
  - dissipation range

The kinetic energy in the inertial range is just transferred into smaller scales without being dissipated. Therefore, the energy-transfer range is the only value to describe the behavior of the inertial range. The dissipation range is characterized by two values: the dissipation rate  $\tilde{\varepsilon}$  and the kinematic viscosity, which is responsible for the dissipation. Based on this approach, the Kolmogorov scales, which describe the smallest structures, only depend on two parameters. A dimension analysis leads to the Kolmogorov time scale (2.18), the Kolmogorov length scale (2.19), and Kolmogorov velocity (2.20).

$$t_{\eta} \equiv \left(\frac{\nu}{\tilde{\varepsilon}}\right)^{1/2} \tag{2.18}$$

$$\eta \equiv \left(\frac{\nu^3}{\tilde{\varepsilon}}\right)^{1/4} \tag{2.19}$$

$$v_{\eta} \equiv \left(\nu \tilde{\varepsilon}\right)^{1/2} \tag{2.20}$$

The large eddies contain the highest amount of kinetic energy. Integral length scale, time scale, and turbulent velocity are described using equation (2.21), Eq. (2.22) and Eq. (2.23).

$$l_t \simeq \frac{k^{3/2}}{\tilde{\varepsilon}} \tag{2.21}$$

$$\tau \simeq \frac{k}{\tilde{\varepsilon}} . \tag{2.22}$$

$$v' = \sqrt{\frac{2}{3}k} \tag{2.23}$$

In Fig. 2.1 it can be seen that the energy is added through turbulent eddies in the integral scale. Energy is transferred through the inertial subrange to successively smaller scales. Finally, the energy is dissipated in the smaller scales through the laminar viscosity.



Figure 2.1: Energy transfer from the integral scale to dissipation scale, according to [71]

Further details on turbulence and turbulence modeling can be found in the literature, for example [15, 18, 34, 36, 60, 71, 72, 74, 76].

## 2.2.2 Averaging of turbulent flows

In all engineering applications high turbulent fluctuations are present, which can not be resolved by the computational grid. For these conditions averaged equations using turbulence models are used. There are two kinds of turbulent flows. One is the stationary flow and the other is the non-stationary flow. For the first case it is sufficient to average the quantities over time. The second approach is to average the quantities of the ensemble (N times the experiment at the same relative time).