

Applying an Extended Flamelet Model for a Multiple Injection Operating Strategy in a Common-Rail DI Diesel Engine

M. Gauding, C. Felsch, B. Kerschgens, A. Vanegas, H. Won and N. Peters

Institut für Technische Verbrennung, RWTH Aachen University

C. Hasse

BMW Group München, previously Institut für Technische Verbrennung, RWTH Aachen University

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ABSTRACT

Subject of this work is the recently introduced extended **Representative Interactive Flamelet (RIF)** model for multiple injections.

First, the two-dimensional laminar flamelet equations, which can describe the transfer of heat and mass between two-interacting mixture fields, are presented. This is followed by a description of the various mixture fraction and mixture fraction variance equations that are required for the RIF model extension accounting for multiple injection events. Finally, the modeling strategy for multiple injection events is described: Different phases of combustion and interaction between the mixture fields resulting from different injections are identified. Based on this, the extension of the RIF model to describe any number of injections is explained.

Simulation results using the extended RIF model are compared against experimental data for a Common-Rail DI Diesel engine that was operated with three injection pulses. Simulated pressure curves, heat release rates, and pollutant emissions are found to be in good agreement with corresponding experimental data. For the pilot injection and the main or post injection, respectively, different ignition phenomena are pointed out and the influence of the scalar dissipation rate on these ignition phenomena is detailly investigated.

INTRODUCTION

The combustion process in modern DI Diesel engines consists of several closely linked subprocesses: injection, spray formation, evaporation, mixing, ignition, and pollutant formation, respectively. The simulation of the combustion process has become an important tool in engine development due to an increasing reliability of the modeling approaches. One major issue is the modeling of the turbulence-chemistry interaction. In many studies, the **Representative Interactive Flamelet (RIF)** model has been applied successfully. A general review of the model and its applications can be found in [2]. Different engines were investigated, ranging from small displacement volumes (300 cm³/cylinder) to marine Diesel (4800 cm³/cylinder) engines, see also [1, 14, 18, 31, 36]. For most of the investigated cases, the injection only consisted of one single pulse. However, injection systems such as Common-Rail are very flexible and allow for splitting the injection into several pulses. A typical application is to use a small pilot injection quantity for noise reduction, a main injection that contains most of the injected mass, and a small post injection quantity for better late stage mixing and soot oxidation. Experiments show that, for example, the ignition delay of the main injection is usually much shorter compared to the case without pilot injection. In most cases, this can be attributed to the transfer of heat and mass between the

mixture fields of pilot and main injection, as the global pressure and temperature rise by the ignition of the pilot injection is usually small. In order to describe this effect, which is different from the auto-ignition process observed for single injection cases, the RIF model and the underlying laminar flamelets equations were extended to account for split injections [16, 17]. Recently, the RIF model was further extended, allowing to account for any number of injections events [7].

In this study, the theory and assumptions underlying the extended RIF model for multiple injections are reviewed. The mixture fraction variable and the two-dimensional flamelet equations are introduced, followed by a description of the coupling of the flamelet solution and the turbulent flow field. Thereby, different phases of mixing and interaction are identified for a typical engine case. After this, the four-cylinder test engine, as well as the investigated operating points, are presented and the numerical setup is described. Following this, simulation results are compared with experimental data, the transfer of heat and mass between interacting mixture fields is investigated in detail, and the applicability of the model is discussed. Finally, the conclusions from the study and the major findings are summarized.

Frequently used definitions, acronyms, and abbreviations, are included at the end of the paper, following the references.

MATHEMATICAL MODEL

THE MIXTURE FRACTION VARIABLE In non-premixed combustion, such as Diesel engine combustion, fuel and oxidizer enter separately into the combustion chamber. The local ratio of the mass flux originating from the fuel feed to the sum of the mass flux from the fuel feed and the oxidizer feed is defined as the mixture fraction Z [29],

$$Z = \frac{\dot{m}_1}{\dot{m}_1 + \dot{m}_2}, \quad (1)$$

where subscript 1 denotes the fuel stream with mass flux $\dot{m}_1$ and subscript 2 denotes the oxidizer stream with mass flux $\dot{m}_2$. For the general case of a multi-feed system with more than one fuel feed, e.g., a multiple injection into a DI Diesel engine, each one of the N fuel feeds can be attributed with one corresponding mixture fraction Z_j . Then, Eq. (1) can formally be extended to

$$Z_j = \frac{\dot{m}_{1j}}{\sum_{n=1}^N \dot{m}_{1n} + \dot{m}_2}, \quad j = 1, \dots, N. \quad (2)$$

The corresponding transport equation reads

$$\rho \frac{\partial Z_j}{\partial t} + \rho v_\alpha \frac{\partial Z_j}{\partial x_\alpha} = \frac{\partial}{\partial x_\alpha} \left(\rho D_Z \frac{\partial Z_j}{\partial x_\alpha} \right), \quad j = 1, \dots, N, \quad (3)$$

where the diffusion coefficient D_Z is chosen to be equal to the thermal diffusivity resulting in a unity Lewis number for all mixture fractions.

Substantial to the flamelet approach is the assumption that the species mass fractions are a function of one or two mixture fractions, depending on the dimensionality of the flamelet equations.

TWO-DIMENSIONAL LAMINAR FLAMELETS The one-dimensional laminar flamelet equations were derived by Peters [27–29]. Hasse and Peters [16] derived two-dimensional laminar flamelet equations accounting for two mixture fractions Z_1 and Z_2 by use of a three-scale asymptotic analysis. These two-dimensional flamelet equations describe the interaction between two mixture fields in the vicinity of stoichiometric mixture.

The two-dimensional flamelet equations for the species mass fractions read

$$\rho \frac{\partial Y_i}{\partial t} - \frac{\rho}{2Le_i} \left(\chi_1 \frac{\partial^2 Y_i}{\partial Z_1^2} + \chi_2 \frac{\partial^2 Y_i}{\partial Z_2^2} \right) - \dot{m}_i = 0, \quad (4)$$

where Le_i is the Lewis number of species i . The scalar dissipation rates are defined by

$$\chi_1 = 2D \left(\frac{\partial Z_1}{\partial x_\alpha} \right)^2, \quad \chi_2 = 2D \left(\frac{\partial Z_2}{\partial x_\alpha} \right)^2. \quad (5)$$

The enthalpy equation in temperature form including radiative heat losses and temporal pressure change is

$$\begin{aligned} \rho \frac{\partial T}{\partial t} - \frac{\rho}{2} \left(\chi_1 \frac{\partial^2 T}{\partial Z_1^2} + \chi_2 \frac{\partial^2 T}{\partial Z_2^2} \right) \\ - \frac{\rho}{2c_p} \frac{\partial T}{\partial Z_1} \left[\chi_1 \frac{\partial c_p}{\partial Z_1} + \sum_{i=1}^{n_s} \frac{c_{p_i}}{Le_i} \left(\chi_1 \frac{\partial Y_i}{\partial Z_1} \right) \right] \\ - \frac{\rho}{2c_p} \frac{\partial T}{\partial Z_2} \left[\chi_2 \frac{\partial c_p}{\partial Z_2} + \sum_{i=1}^{n_s} \frac{c_{p_i}}{Le_i} \left(\chi_2 \frac{\partial Y_i}{\partial Z_2} \right) \right] \\ = \frac{1}{c_p} \left(\frac{\partial p}{\partial t} - \dot{q}_r - \sum_{i=1}^{n_s} h_i \dot{m}_i \right). \end{aligned} \quad (6)$$

The solution of Eqs. (4) and (6) requires a closed description of the scalar dissipation rates in (Z_1, Z_2) -space.

The stationary solution for χ_1 reads

$$\begin{aligned}\chi_1(Z_1, Z_2) &= \frac{a_1}{\pi} (1 - Z_2)^2 \\ &\times \exp\left(-2[\operatorname{erfc}^{-1}(2Z_1/(1 - Z_2))]^2\right) \\ &= f_{\operatorname{erfc},1}(Z_1, Z_2),\end{aligned}\quad (7)$$

where a_1 denotes the compressive strain rate [13]. The equation for χ_2 is completely analogous.

The solution domain for the two-dimensional flamelet equations in (Z_1, Z_2) -space is a unit triangle as the sum of both mixture fractions cannot exceed one. To avoid numerical difficulties, a transformation to a unit square, reading

$$Z = Z_1 + Z_2, \quad y = Z_2/(Z_1 + Z_2), \quad (8)$$

is applied. This is schematically shown in Fig. 1. Transforming Eq. (4) for the species mass fractions into (Z, y) -space yields

$$\begin{aligned}\rho \frac{\partial Y_i}{\partial t} - \frac{\rho \chi_1}{2Le_i} \left(\frac{\partial^2 Y_i}{\partial Z^2} - 2\frac{y}{Z} \frac{\partial^2 Y_i}{\partial Z \partial y} + 2\frac{y}{Z^2} \frac{\partial Y_i}{\partial y} \right. \\ \left. + \frac{y^2}{Z^2} \frac{\partial^2 Y_i}{\partial y^2} \right) - \frac{\rho \chi_2}{2Le_i} \left(\frac{\partial^2 Y_i}{\partial Z^2} + 2\frac{1-y}{Z} \frac{\partial^2 Y_i}{\partial Z \partial y} \right. \\ \left. - 2\frac{1-y}{Z^2} \frac{\partial Y_i}{\partial y} + \frac{(1-y)^2}{Z^2} \frac{\partial^2 Y_i}{\partial y^2} \right) - \dot{m}_i = 0.\end{aligned}\quad (9)$$

The enthalpy equation in temperature form in (Z, y) -space reads

$$\begin{aligned}\rho \frac{\partial T}{\partial t} - \frac{\rho \chi_1}{2Le_i} \left(\frac{\partial^2 T}{\partial Z^2} - 2\frac{y}{Z} \frac{\partial^2 T}{\partial Z \partial y} + 2\frac{y}{Z^2} \frac{\partial T}{\partial y} \right. \\ \left. + \frac{y^2}{Z^2} \frac{\partial^2 T}{\partial y^2} \right) - \frac{\rho \chi_2}{2Le_i} \left(\frac{\partial^2 T}{\partial Z^2} + 2\frac{1-y}{Z} \frac{\partial^2 T}{\partial Z \partial y} \right. \\ \left. - 2\frac{1-y}{Z^2} \frac{\partial T}{\partial y} + \frac{(1-y)^2}{Z^2} \frac{\partial^2 T}{\partial y^2} \right) \\ - \frac{\rho}{c_p} \left(\frac{\partial T}{\partial Z} - \frac{y}{Z} \frac{\partial T}{\partial y} \right) \left[\sum_{i=1}^{n_s} \frac{c_{p_i}}{Le_i} \frac{\chi_1}{2} \left(\frac{\partial Y_i}{\partial Z} - \frac{y}{Z} \frac{\partial Y_i}{\partial y} \right) \right. \\ \left. + \frac{\chi_1}{2} \left(\frac{\partial c_p}{\partial Z} - \frac{y}{Z} \frac{\partial c_p}{\partial y} \right) \right] - \frac{\rho}{c_p} \left(\frac{\partial T}{\partial Z} + \frac{1-y}{Z} \frac{\partial T}{\partial y} \right) \\ \times \left[\sum_{i=1}^{n_s} \frac{c_{p_i}}{Le_i} \frac{\chi_2}{2} \left(\frac{\partial Y_i}{\partial Z} + \frac{1-y}{Z} \frac{\partial Y_i}{\partial y} \right) \right. \\ \left. + \frac{\chi_2}{2} \left(\frac{\partial c_p}{\partial Z} + \frac{1-y}{Z} \frac{\partial c_p}{\partial y} \right) \right] \\ = \frac{1}{c_p} \left(\frac{\partial p}{\partial t} - \dot{q}_r - \sum_{i=1}^{n_s} \dot{m}_i h_i \right).\end{aligned}\quad (10)$$

The new variables Z and y correspond to the overall mixture fraction Z and a mixing parameter y , respectively. All equations are transformed and solved in this new coordinate system. The corresponding numerical solver will be referred to as the flamelet code in the following.

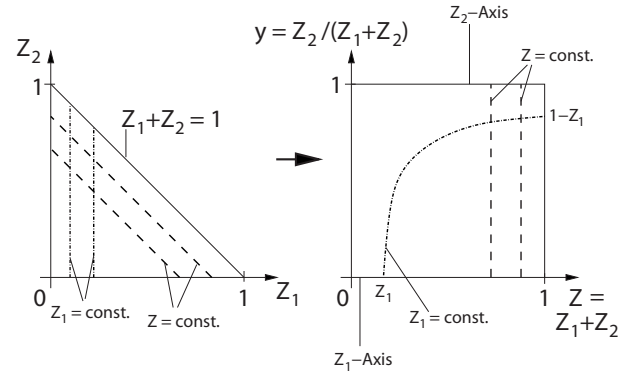


Figure 1: Coordinate transformation from (Z_1, Z_2) -space to (Z, y) -space

CFD CODE The CFD code used in this work is AC-FluX (formerly known as GMTEC), a flow solver based on Finite Volume methods [8] that employs unstructured, mostly hexahedral meshes. AC-FluX solves for the partial differential equations for continuity, the Navier-Stokes equations, an equation for the total enthalpy, and two equations to account for the turbulence (k-epsilon-model). The spray liquid phase is coupled to the gas phase via source terms and modeled using the Lagrangian particle method. AC-FluX is documented by Khalighi et al. [21] and by Ewald et al. [6]. A detailed description of the spray modeling in AC-FluX can be found in [34].

For the coupling of the CFD and the flamelet code, additional transport equations for each mean mixture fraction $\tilde{Z}_j$ and its variance $\tilde{Z}_j'^2$ have to be solved. This yields

$$\frac{\partial}{\partial t} (\bar{\rho} \tilde{Z}_j) + \frac{\partial}{\partial x_\alpha} (\bar{\rho} \tilde{v}_\alpha \tilde{Z}_j) = \frac{\partial}{\partial x_\alpha} \left(\frac{\bar{\rho} \nu_t}{Sc_{\tilde{Z}_j}} \frac{\partial \tilde{Z}_j}{\partial x_\alpha} \right) + \bar{\rho} \tilde{S}_j \quad (11)$$

with $\tilde{S}_j$ denoting the evaporation source term of fuel stream j and

$$\frac{\partial}{\partial t} \left(\bar{\rho} \widetilde{Z_j''^2} \right) + \frac{\partial}{\partial x_\alpha} \left(\bar{\rho} v_\alpha \widetilde{Z_j''^2} \right) = \frac{\partial}{\partial x_\alpha} \left(\frac{\bar{\rho} \nu_t}{Sc_{\widetilde{Z_j}}} \frac{\partial \widetilde{Z_j''^2}}{\partial x_\alpha} \right) + 2 \underbrace{\frac{\bar{\rho} \nu_t}{Sc_{\widetilde{Z_j}}} \left(\frac{\partial \widetilde{Z_j}}{\partial x_\alpha} \right)^2}_{\text{Production}} - \underbrace{\bar{\rho} \widetilde{\chi_j}}_{\text{Dissipation}} + \bar{\rho} S_j^+ - \bar{\rho} S_j^- \quad (12)$$

with $\widetilde{\chi_j}$ being the Favre-averaged scalar dissipation rate of fuel stream j . The source terms $\bar{\rho} S_j^+$ and $\bar{\rho} S_j^-$ in Eq. (12) accounting for droplet evaporation will be neglected in the following. According to Gill et al. [10], they contribute only 5 % in comparison to the production and dissipation source term.

In addition to the mixture fraction equations for each fuel stream j , equations for the total mean mixture fraction $\widetilde{Z}$, being the sum of all mean mixture fractions $\widetilde{Z_j}$, and its variance $\widetilde{Z''^2}$ are solved. Moreover, at the time when a new fuel feed j enters the combustion chamber, equations for a mean mixture fraction accounting for the sum of all previous $j - 1$ fuel streams/mean mixture fractions and its variance are solved. For example, considering an injection strategy with three pulses (pilot, main, and post injection), equations for a mean mixture fraction accounting for the sum of pilot and main injection and its variance are solved when the post injection first enters the combustion chamber. Solving these equations is necessary for the modeling strategy for multiple injections, which is discussed below.

RIF MODEL

Interaction between CFD Code and Flamelet Code

The RIF model interactively couples the solution of the turbulent flow field with the instantaneous flamelet solution at every CFD time step.

The CFD code solves the three-dimensional equations for the flow, the turbulence, the total enthalpy, all mixture fractions, and their variances described above. The flamelet parameters $\widehat{\chi}_{st,1}$, $\widehat{\chi}_{st,2}$, and $\widehat{p}$ are calculated from the turbulence and mixture field and are then passed to the flamelet code. During one time step of the CFD code, the flamelet code solves the unsteady flamelet equations with time steps that can be much smaller. In this way, the time scales of the fluid dynamics and the chemistry are decoupled. The flamelet code calculates the species mass fractions $Y_i(Z, y, t)$. Turbulent mean values in the CFD code are obtained by a PDF integration. The β -PDF is used in this work. The mean species mass fractions $\widetilde{Y}_i(x_\alpha, t)$ and the mean total enthalpy $\widetilde{h}$ are then used to iteratively compute the mean temperature $\widetilde{T}$ in the CFD code. Figure 2 illustrates the procedure.

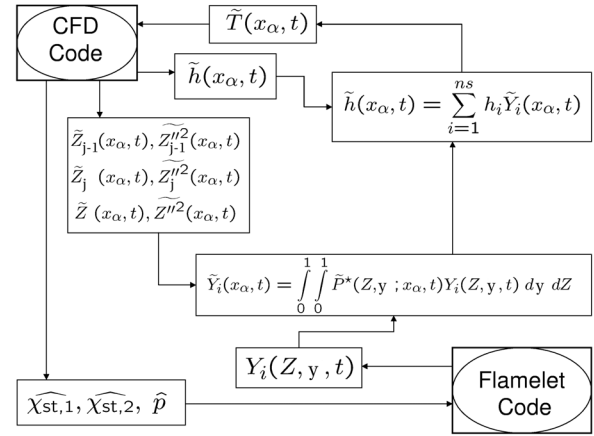


Figure 2: Structure of the Representative Interactive Flamelet concept for multiple injections

In the following, the modeling strategy to account for multiple injections within the flamelet framework will be presented for an operating condition with three injections. There is no conceptual difference for operating conditions with more than three injections.

Multiple Injections A common strategy when using multiple injections is to use a small pilot injection quantity, a main injection, and a post injection quantity. The pilot injection leads to a smoother pressure rise when the main injection starts to burn and thus mainly aims at reducing engine roughness. The post injection improves late stage mixing and can reduce soot emissions significantly. A typical injection rate obtained experimentally for a passenger car engine under part load conditions with a pilot, a main, and a post injection is shown in Fig. 3.

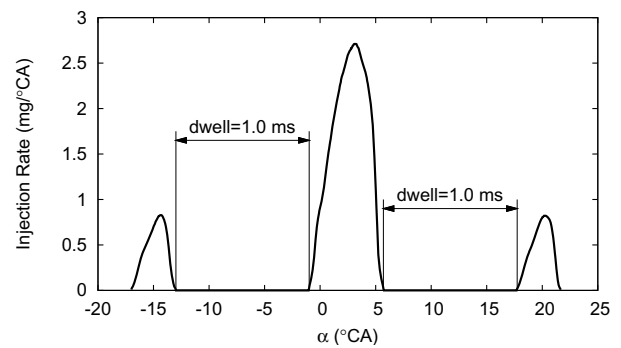


Figure 3: Measured injection rate for GM FIAT engine for a part load case; pilot, main, and post injection

Start of injection (SOI) of the pilot quantity is at -17.0 degs. CA after top dead center (aTDC), the end of the pilot injection (EOI) is at -13.0 degs. CA aTDC. After a dwell time of 1.0 ms, the main injection enters the com-

bustion chamber at -1.0 degs. CA aTDC and lasts until 5.7 degs. CA aTDC. The dwell time between main and post injection is 1.0 ms. The post injection lasts from 17.7 degs. CA aTDC until 21.7 degs. CA aTDC.

For cases with three injections, five phases can be distinguished:

1. Start of the pilot injection until start of main injection.
2. Early phase of main injection, the two mixture fields are spatially separated and not in contact. No direct interaction, such as heat and mass transport between the reactive structures, associated with the mixture fields takes place.
3. Late phase of main injection, the mixture fields have merged, interaction between the reactive structures takes place; heat and mass are exchanged.
4. Early phase of post injection, the mixture field of the post injection is spatially separated from the mixture fields of pilot and main injection.
5. Final phase, the mixture field of the post injection has merged with mixture fields of the pilot and main injection, interaction between the reactive structures takes place; heat and mass are exchanged.

For the distinction of the phases, time separation regarding the ensemble averaged point of view is assumed. The different phases are further illustrated in Fig. 13 and discussed in detail in the associated section.

Modeling Strategy for Multiple Injections The first phase of the five phases identified above can be described by the original flamelet model [2] with one corresponding mixture fraction; the flamelet equations are one-dimensional in mixture fraction space.

As long as the structures are separated in physical space, no interaction in flamelet space is allowed to take place. This is also characteristic for the second phase. Two independent one-dimensional flamelets with different initial times are solved. The flamelet parameters are computed according to the original model with the extension of having one representative scalar dissipation rate per mixture fraction. For the second phase, the respective mixture fractions are $Z_1 = Z_{\text{pilot inj.}}$ and $Z_2 = Z_{\text{main inj.}}$ with initial times corresponding to the individual starts of injection.

It is important to decide when two structures start to interact. For this, the mixture field is investigated by looking at the domain averaged two-dimensional β -PDF in (Z, y) -space in the vicinity of stoichiometric mixture. The

β -PDF has shown to be a good approximation of homogeneous, isotropic turbulence [11, 12] and jet-diffusion flames [20]. Girimaji [11] generalized the β -PDF to multiple scalars. This PDF used in this work is formulated for the three scalars Z_1 , Z_2 , and oxidizer. The PDF is also transformed to (Z, y) -space using standard techniques for probability density functions, see e.g. [26]. An interaction coefficient $I_{1,2}$ is defined as

$$I_{1,2} = \frac{\int_V \rho \int_{\varepsilon}^{1-\varepsilon} \int_{Z_{st}-\Delta Z}^{Z_{st}+\Delta Z} \tilde{P}^*(Z, y; x_\alpha, t) dZ dy dV'}{\int_V \rho \int_0^1 \int_{Z_{st}-\Delta Z}^{Z_{st}+\Delta Z} \tilde{P}^*(Z, y; x_\alpha, t) dZ dy dV'} \quad (13)$$

where $\tilde{P}^*(Z, y; x_\alpha, t)$ denotes the two-dimensional β -PDF in (Z, y) -space. ΔZ is of the order of the flame zone thickness in mixture fraction space, and ε as a small number defines the separation of the inner part and the asymptotic limit of pure mixture of either Z_1 or Z_2 . By use of ε and ΔZ , an interaction domain for both mixture fields associated with the mixture fractions Z_1 and Z_2 is defined. As long as no interaction takes place, the mixture is either located at $y = 0$ or at $y = 1$. As the two fields start to merge, the inner part $0 < y < 1$ is also represented. The interaction starts for small values of the interaction coefficient $I_{1,2}$, as experimental investigations showed the triggering of the burning of the main injection shortly after the two mixture fields get into contact [22]. For $I_{1,2}$, a threshold value of 0.4 was chosen in this work. However, when the two mixture fields get into contact, the interaction coefficient $I_{1,2}$ rapidly increases. For this reason, the influence of the exact choice of the threshold value is small when varying it between 0.1 and 0.5.

When structures start to interact, the flamelet equations given in Eqs. (4) and (6) transformed in (Z, y) -space are solved in the flamelet code, which corresponds to the third phase. The mean species mass fractions are then obtained by a two-dimensional β -PDF integration in each CFD cell according to

$$\tilde{Y}_i(x_\alpha, t) = \int_0^1 \int_0^1 \tilde{P}^*(Z, y; x_\alpha, t) Y_i(Z, y, t) dZ dy. \quad (14)$$

The mixture fields of pilot and main injection are interacting during the third phase. After a short period of heat and mass transfer between the two reacting structures, a homogeneous solution has established itself in the second flamelet dimension (y -direction). This is discussed in detail within the "Results and Discussion" section. At this point, the two-dimensional flamelet can be collapsed to a one-dimensional flamelet according to