Three Dimensional Modeling of DI Diesel Engine Combustion using a Flamelet Concept

C. Hasse, N. Peters

Institut für Technische Mechanik
RWTH Aachen
Templergraben 64
52056 Aachen
Germany
c.hasse@itm.rwth-aachen.de

Abstract

Combustion and pollutant formation in a DI-Diesel engine are numerically investigated using the **E**ulerian **P**article **F**lamelet **M**odel (EPFM). A surrogate fuel consisting of n-decane (70% liquid volume fraction) and α-methylnaphthalene (30% liquid volume fraction) is used in the simulation. Results are compared to experimental data that has been obtained using real diesel fuel. The effect of multiple flamelets on the simulation of the auto-ignition process and the pollutant formation is shown and a converging behavior of the model with respect to the number of flamelets is found.

Introduction

Numerical simulation of diesel engine combustion has become an important tool in engine development. One major issue in modeling of turbulent reactive flows is the interaction of turbulence and chemistry. One successful way to model this interaction is the use of the Representative Interactive Flamelet (RIF) model. The RIF model describes all phases of diesel engine combustion and therefore there is no need to use separate submodels for ignition or diffusive burning. It allows to use detailed reaction schemes which include submechanisms for all major pollutants such as NOx or soot. The RIF model has been recently extended to a multiple flamelet model which is called Eulerian Particle Flamelet Model (EPFM). Each representative flamelet is represented by an eulerian particle having its own time history. These particles are convected through the flow field and an equation for the probability of finding a particle at a certain location and time has been derived on the basis of a Pdf transport equation. Using multiple flamelets allows to account for spatial variations of the scalar dissipation rate which is especially important during the ignition phase.

Laminar Flamelets

The laminar flamelet equations have been derived by Peters [1, 2], where a local coordinate transformation and boundary layer arguments were used. In a recent publication [3] he demonstrates the derivation of the flamelet equations applying a two scale asymptotic analysis. The resulting equations are:

$$\rho\frac{\partial T}{\partial t}-\rho\frac{\chi}{2}\frac{\partial^2 T}{\partial Z^2}-\rho\frac{\chi}{2c_p}\frac{\partial T}{\partial Z}\frac{\partial c_p}{\partial Z}-\sum_i^N\rho\frac{\chi}{2\mathrm{Le}_i}\frac{c_{p_i}}{c_p}\frac{\partial Y_i}{\partial Z}\frac{\partial T}{\partial Z}$$

$$+\frac{1}{c_p}\sum_i^N \dot{m}_i h_i - \frac{1}{c_p}\frac{\partial p}{\partial t} = 0, \tag{1}$$

and

$$\rho\frac{\partial Y_i}{\partial t} - \rho\frac{\chi}{2\mathrm{Le}_i}\frac{\partial^2 Y_i}{\partial Z^2} - \dot{m}_i = 0\,. \tag{2}$$

In these equations N denotes the number of chemical species, p the pressure, c_{p_i}, $\dot{m}_i$, h_i, Y_i, p, Le_i are the heat capacities at constant pressure, the chemical production rates, the enthalpies, the mass fractions of the chemical species i, the pressure, and the Lewis number of species i, respectively.

Characteristic for Eqs.(1) and (2) is that after the transformation into phase space (mixture fraction) the convective terms disappear. Since all scalars are convected with the same velocity in physical space no relative convective velocities exist between the mixture fraction and the other scalars such as species mass fractions or temperature. The coupling of the equations in phase space to the flow field in physical space is now established by the pressure p and a new parameter, which is the scalar dissipation rate,

$$\chi = 2D_Z\left(\nabla Z\right)^2\,, \tag{3}$$

occurring in all the terms in Eqs.(1) and (2) that contain derivatives in phase space. Here D_Z denotes the diffusion coefficient of the mixture fraction. The scalar dissipation rate represents the strain effects of the flow field on the transport of the scalars in phase space.

Unsteady flamelets were used first by Mauss et al. [4] to simulate flamelet extinction and re-ignition in a steady turbulent jet diffusion flame. In a Diesel Engine the turbulent flow and mixture fields are non-homogeneous. Especially, the scalar dissipation rate will vary spatially and with time. The history of the scalar dissipation rate and the boundary conditions determine the solution of a flamelet, with the consequence that different flamelet histories must be calculated if these parameters vary too much in the physical domain.

RIF Concept

The RIF-concept for a single flamelet has been extensively described [1–3, 5] and applied [6–12]. Therefore, only a short summary of the model is given here. In the framework of the RIF-concept the solution of the three-dimensional flow field is decoupled from the solution of the chemistry for which the flamelet equations are solved. The interaction between the CFD-code and the flamelet code is shown schematically in Fig. 1. The CFD-code solves the three-dimensional equations for the flow, the turbulence, the enthalpy, the mixture fraction and its variance. The flamelet parameters $\widehat{\chi}_{st}, \widetilde{p}, Z_l$ and Z_r 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 $Y_i(Z)$ from which the mean values are computed by a Pdf integration. The mean temperature is calculated by an iterative procedure is passed to the CFD code. Recently this concept has been extended to more than one flamelet and a complete derivation is given in [13].

Results

We present results for an engine that is derived from an Audi V6 2.5 liter running under part load conditions. This research engine is equipped with a modern Common-Rail injection system and a piezo-injector. The

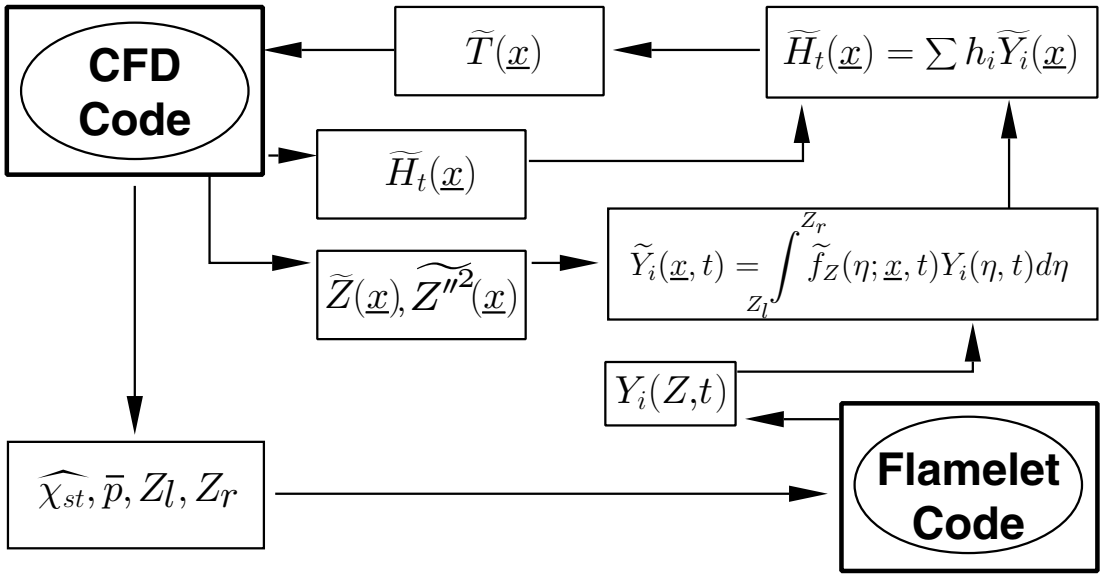

Figure 1: Structure of the Representative Interactive Flamelet concept.

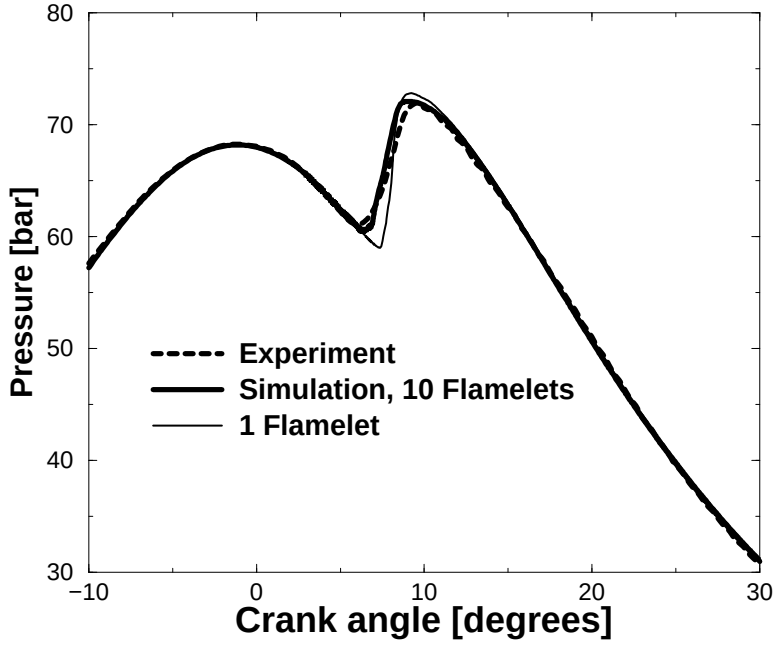

Figure 2: Comparison between experimental and simulated pressure curves. Simulations with 1 and 10 flamelets.

experiments were carried out using regular diesel fuel. In the simulations a detailed kinetic mechanism for the IDEA model fuel was used. The IDEA fuel is a mixture of n-decane and $\alpha-$methylnaphathalene and it has been shown to reproduce all major characteristics of diesel such as ignition delay, heat release and pollutant formation.

Figure 2 compares the experimental pressure with the simulation results. Computations are shown for 1 and 10 flamelets. The curve for 10 flamelets follows nicely the experimental curve. On the other hand the computation for 1 flamelet shows delayed ignition. By using one flamelet it is only possible to describe the mean ignition delay in the combustion chamber. The use of multiple flamelets allows to take into account spatial differences of the scalar dissipation rate. If the variations of the scalar dissipation rate at stoichiometric mixture within one flamelet exceed a certain limit, the flamelet is subdivided. A detailed description of this process

and the criteria that lead to subdivision are given in [14]. This subdivision of flamelets is shown in Fig. 3. At

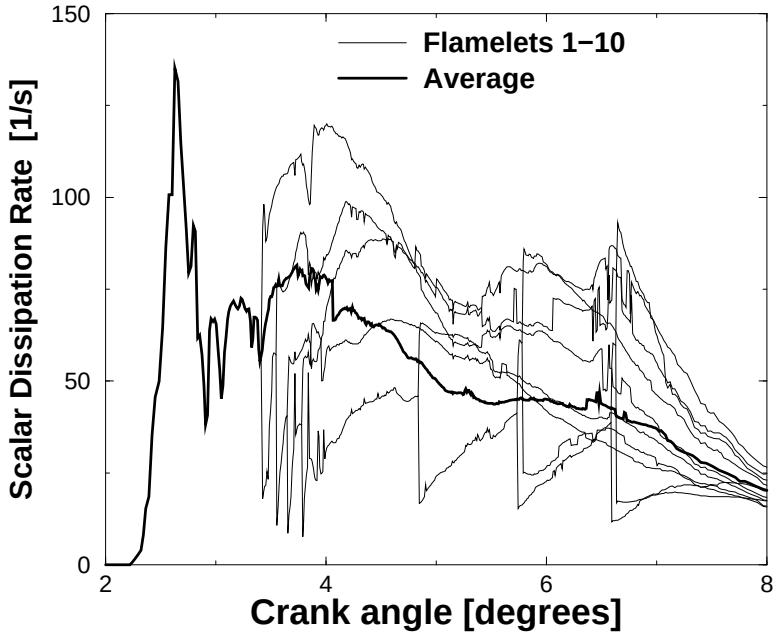

Figure 3: Scalar dissipation rates for the baseline case, each time a flamelet is subdivided a new curve is added.

the beginning only one flamelet is representative for the whole domain. At 3.4° CA the variations of the scalar dissipation rate within the first and only flamelet at that time have become exceed a prescribed limit, thus the flamelet is subdivided into two flamelets. In the following new flamelets are created as need arises. The first flamelet ignites at 6.4° CA. Computations for 20 flamelets have also been carried out. The pressure curve is almost indistinguishable from the curve for 10 flamelets therefore it is not included in Fig. 2 but the results for the pollutants NO_x and soot are included in Table 1.

	NO_x [ppm]	Soot [mg/m^3]
Experiment	324	SZ[Bosch]=0.27
1 Flamelet	373	0.31
10 Flamelets	335	0.46
20 Flamelets	333	0.46

Table 1: Pollutant concentrations in the exhaust gas

References

[1] Peters N., *Prog. Energy Combust. Sci.* 10:319–339 (1984).

[2] Peters N., *Proc. Combust. Inst.*, vol. 21, The Combustion Institute, Pittsburgh, 1986, pp. 1231–1250.

[3] Peters N., *Turbulent Combustion*, Cambridge University Press, 2000.

[4] Mauss F., Keller D., and Peters N., *Proc. Combust. Inst.*, vol. 23, The Combustion Institute, Pittsburgh, 1990, pp. 693–698.

[5] Pitsch H., *Modellierung der Zündung und Schadstoffbildung bei der dieselmotorischen Verbrennung mit Hilfe eines interaktiven Flamelet-Modells*, Ph.D. thesis, RWTH Aachen, 1997.

[6] Pitsch H., Wan Y.P., and Peters N., *Paper No. SAE 952357* .

[7] Pitsch H., Barths H., and Peters N., *Paper No. SAE 962057* .

[8] Barths H., Pitsch H., and Peters N., Sheh M. (ed.), *Proceedings of the 3rd International Conference on High Performance Computing in the Automotive Industry*, 1977.

[9] Barths H., Antoni C., and Peters N., *Paper No. SAE 982459* .

[10] Barths H., Pitsch H., and Peters N., *Oil & Gas and Technology-Rev*, vol. 54, IFP, 1999, pp. 23–244.

[11] Hasse C., Barths H., and Peters N., *Paper No. SAE 1999-01-3547* .

[12] Hergart C.A., Barths H., and Peters N., *Paper No. SAE 1999-01-3550* .

[13] Barths H., Hasse C., Bikas G., and Peters N., *Proc. Combust. Inst.*, vol. 28, The Combustion Institute, Pittsburgh, 2000, p. accepted for publication.

[14] Barths H., Hasse C., and Peters N., *Journal of Engine Research* 1:249–267 (2000).