# Aspects of 0D and 3D Modeling of Soot Formation for Diesel Engines

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### **1** Introduction

Accurate prediction of soot emissions from Diesel engines is still a challenging task due to the complexity of physical and chemical processes involved in soot formation and oxidation. This results in a number of modeling assumptions that are needed to describe the complex chemistry of soot formation and oxidation, together with the turbulent flow and chemistry interactions.

Among the available methods for calculating chemistry–flow interaction, the interactive flamelet approach is a possible choice [1-3]. The advantage of that approach is that no species transport equations are needed in the 3D CFD code. This makes the method computationally efficient and allows for the application of complex chemical reaction mechanisms for calculating the combustion processes [3]. Furthermore, the interactive flamelet formulation facilitates the use of a detailed kinetic soot model for prediction of soot formation in turbulent diffusion flames or Diesel engines [4-6]. It is however questionable if the chemical time scales of soot formation allow for interactive flamelet modeling; i.e. if the concentration of soot in the burned gas is only dependent on the local mixture. Also temperature effects induced by the heat loss to the walls cannot be considered.

To overcome the difficulties with the interactive flamelet model, a flamelet library approach has been proposed. First, it was adapted to a laminar diffusion flame [7] and then extended to a turbulent diffusion flame [8]. In this approach the source terms of the soot formation processes were tabulated, rather than the soot amount in the steady state flamelet. Then a transport equation for soot volume fraction was introduced. In [9] we used the fact that the flamelet library based soot model was independent of the combustion model. The local enthalpy was just needed to select the flamelet from the library. This allowed implementing the model into CFD codes for engineering applications [10, 11]. In reference [11] a sectional method was used to calculate the soot particle size distribution functions (PSDF), while in [12] the method of moments was utilized.

In this work, using a 0D Probability Density Function (PDF) based direct injection stochastic reactor model (DI-SRM) from [12], we provide a plausibility study for assumptions made for the flamelet soot source term model, which was published before [7–9, 11]. The most crucial assumptions in this model are: 1) it is possible to provide gas phase species, necessary to calculate source terms of soot formation (particle inception, surface growth and oxidation) from a stationary flamelet library,

and 2) the time scale for soot formation is too long to allow the application of transient interactive flamelet models. From the 0D DI-SRM, which allows calculating the gas phase chemistry using detailed kinetics and the soot formation process in detail, we calculate the joint PDF's of species concentrations, temperature, reaction progress and the mixture fraction. This enables investigation of the underlying assumptions of stationary and transient flamelet models under Diesel engine conditions. The 3D CFD calculations are used to verify the mixing time history, which we apply in the 0D DI-SRM.

## 2 Numerical Models

The 0D DI-SRM and 3D CFD are two numerical models used for the presented analysis. Details of these models are beyond the scope of this extended abstract. We present only basic information for completeness.

## DI-SRM

The DI-SRM is a probability density function (PDF) model for simulating the interaction of chemistry and flow in engines within a 0D framework. The DI-SRM considers gas inside the cylinder as an ensemble of particles that can mix with each other and exchange heat with the walls. The particles are defined by chemical composition, temperature and equal mass. These scalars determine composition of the gas mixture and are considered as random variables that can vary within the cylinder. They are described with probabilities using PDFs. From the joint distributions for species concentration and temperature the reaction progress is calculated. Subsequently, using species and energy conservation equations, the global engine quantities such as mean pressure and temperature are calculated. For the DI Diesel engine the model accounts for convective heat loss, volume changes due to piston motion, and fuel injection. The effects of turbulence are captured by simulating the mixing process between the particles; the mixing process is simulated using the particle–interaction model and applying the time dependent turbulent mixing time as proposed in [14] and explained in detail in [15]. More detailed information about the DI-SRM can be found in [12].

## 3D CFD

All CFD calculations have been extracted from [16]. They were performed with the commercial CFD package STAR-CD. The combustion model applied in that study was the 7-species-PDF-Timescale combustion model [17]. Soot formation was calculated using the method of moments [18]. The source terms of particle inception, surface growth and oxidation have been tabulated in a laminar flamelet library [11]. The dimension of the library in temperature, pressure, EGR and scalar dissipation was chosen such that their variations in a Diesel engine conditions were covered. The data are presented for verification of the soot modeling work in the DI-SRM.

## Kinetics of Combustion and Soot Modeling

A skeleton reaction mechanism for n-heptane [19] has been used to simulate emission formation within the DI-SRM and to generate the flamelet library for 3D CFD calculation. The mechanism contains 121 species and 973 reactions, including backwards reactions. Details of the employed kinetic soot model can be found in [20].

## 3 Simulation Test Case Setup

Simulation results refer to the direct injection Diesel engine presented in [16]. Based on this data, engine specifications listed in Table 1 and Table 2 define the analyzed operating condition. All the experimental and CFD results presented in this work have been extracted from [16].

Table 2: Engine operating condition

Table 1: Engine basic specification

Engine Type	DI Diesel	Parameter	Value
Bore [mm]	83	Engine speed [min <sup>-1</sup> ]	2000
Stroke [mm]	99	BMEP [bar]	14
Compression ratio [-]	16.2	EGR [-]	0.27
Fuel	Diesel	Lambda	1.33

#### **4** Simulation Results

### DI-SRM and 3D CFD Models Validation

The DI-SRM is a 0D model and thus not able to predict the mixing time scales occurring in engines. The mixing process depends mainly on the turbulent flow in the cylinder and the spray. These processes are geometry dependent and thus have 3D character. To overcome this difficulty, the mixing time for the DI-SRM is considered as a modeled parameter as in [14-15]. The parameters determining mixing time history are obtained using optimization technique introduced in [13].

The pressure and rate of heat release (ROHR) histories calculated by the DI-SRM match the 3D CFD results and the experimental data with high accuracy (Fig. 1a). The optimized for the DI-SRM mixing time matches the 3D CFD results qualitatively (Fig.1b). Note that a conditioning of the mixing time in mixture fraction will be necessary to discuss absolute numbers of the mixing time.



Figure 1. In-cylinder pressure and ROHR history from the DI-SRM compared to 3D CFD results and experimental data (a). Optimized mixing time history for the DI-SRM compared to the 3D CFD result (b) (experimental and CFD results extracted from [16])

The CFD profile was calculated over the combustion chamber as the ratio of the turbulent kinetic energy and its dissipation. Thus it denotes the turbulent mixing time induced by the velocity. In contrast, the mixing time for the DI-SRM represents the turbulent molecular mixing induced by the scalars. These two time scales are related by the mixing time constant  $c_{\phi}$  which for the operating point under consideration is in the range 0.14–1.30 and these values seem plausible (see, e.g. [21]). With such defined mixing time the SRM can be interpreted as a mean representative stochastic reactor model. This concept might be compared to calculations with a single representative interactive flamelet. We conclude at this point that it is possible to analyze results from the SRM in terms of the flamelet theory.

### Plausibility Study Using the DI-SRM

Figure 2 visualizes profiles for  $C_2H_2$ , OH, NO and the first moment of the soot particle size distribution function in mixture fraction space at 15 CAD and 30 CAD after top dead center (ATDC). These positions correspond to soot formation and oxidation phases respectively (see Fig. 4a). The species were selected since they represent different chemical time scales.

Following the Hydrogen Abstraction Carbon Addition (HACA) mechanism for soot surface growth,  $C_2H_2$  is the most important growth species, while OH is the most important species for soot oxidation. From Fig. 2 it is evident that the flamelet structure is very well established by the SRM calculation. The NO species is reacting on the slowest chemical time scale and presents a wide spread of data points. For NO the flamelet approximation might be questionable since a large variation of the NO mass fraction exists for each coordinate in mixture fraction space and there is no simple relation between mixture fraction and NO mass fraction.



Figure 2. Calculated by the DI SRM mole fractions of  $C_2H_2$ , OH, NO and first moment of the soot particle size distribution function in mixture fraction space at 15 CAD and 30 CAD ATDC



Figure 3. Rate of soot formation via  $C_2H_2$  and rate of oxidation via OH as functions of mixture fraction at 15 CAD and 30 CAD ATDC

Hydroxyl is the fastest reacting species and shows a perfect one dimensional structure. In contrast to that, the calculated first moment of the soot particle size distribution function exhibits more spread and does not manifest a one dimensional flamelet-like structure. It seems that due to the distribution of the soot moments (in magnitude for the same mixture fraction coordinate) it can be more accurate to use the rates of soot formation together with flamelet models, than to calculate the soot concentrations by the interactive flamelet model. This is partially proved by looking at the calculated soot source terms

(particle inception, surface growth and oxidation) in Fig. 3; the flamelet structure is better established for the source terms than for the calculated first moment of the soot particle size distribution function.

### Application of the Emission Source Term Model

Figure 4a and Fig. 4b present performance of the DI-SRM and the 3D CFD model in predicting soot formation. Both models use the same chemical schemes for gas-phase (n-heptane) and Polycyclic Aromatic Hydrocarbons (PAH) chemistry in the soot model (see also Sec. 2). In Ref. [16] the assumptions concerning use of PAH chemistry and n-heptane as Diesel surrogate are discussed.

In Fig. 4a the time history of the normalized soot mass as calculated by the DI-SRM and the 3D CFD model is shown. The integral of the soot formation process is very similar for both models. However, the soot oxidation is slightly different. At first soot oxidation appears faster in the CFD calculation but towards the end of the cycle soot oxidation is frozen in CFD, while the process continues in the DI-SRM calculation. The freezing of the soot oxidation might be explained by the missing tabulation entries for the expansion stroke. The missing library entries result from the decrease in enthalpy, caused by the pressure work performed by the engine. The faster oxidation in the beginning of the soot oxidation phase can be explained by the circumstance that the flamelet library based soot model utilizes mean particle surface areas. This is necessary, since the profiles of the soot moments in the mixture fraction are unknown.



Figure 4. Rates of soot formation and oxidation from CFD and DI-SRM compared to rate (a). Soot prediction by the CFD for different values of lambda (b) (experimental and CFD results extracted from [16])

Figure 4b demonstrates applicability of the flamelet library for the source terms of soot formation. Experiments and calculations are shown for a variation of the EGR between 0% and 27%, which corresponds to variation in lambda between 1.89 and 1.33. The results indicate that the flamelet library based model follows the trend of the experiment with high accuracy.

### 5 Summary

This paper reports on the utilization of two different models for simulating combustion and emission formation in Diesel engines. A 0D DI-SRM is used to describe the interaction of chemistry and flow by a PDF approach. This model has low cost of CPU and allows for direct application of detailed kinetic models for fuel oxidation and emission formation. On the other hand a 3D CFD model is employed that describes combustion using a PDF-time scale model. Soot formation is modeled by the help of a flamelet library model for the source terms of soot formation. Despite the differences between the models, they can be used to make approximations made by both models plausible.

The 0D model was shown to mimic the turbulent mixing process in a Diesel engine. Since the 0D model allows for the application of detailed chemistry, it is able to calculate for example the profiles of species and emissions in the mixture fraction coordinate. Hence, the model can be used to

demonstrate how fast flamelet structures for the different species are reached. It was found that species reacting on short time scales show profiles which agree very well with the flamelet theory. Emissions like NO or soot however show a broad variation of the data, when plotted as a function of mixture fraction. This casts doubt on the calculation of emissions from representative interactive flamelets. One possible alternative is the application of source term libraries. Benefits of this model are: 1) it is not limited to a certain combustion model; 2) the demand of the model on CPU time is low, since chemistry does not need to be evaluated during the execution of the program. Instead a flamelet library can be calculated prior to the CFD calculation.

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