

Soot Simulation under Diesel Engine Conditions Using a Flamelet Approach

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ABSTRACT

The subject of this work is 3D numerical simulations of combustion and soot emissions for a passenger car diesel engine. The CFD code STAR-CD version 3.26 [1] is used to resolve the flowfield. Soot is modeled using a detailed kinetic soot model described by Mauss [2]. The model includes a detailed description of the formation of polyaromatic hydrocarbons. The coupling between the turbulent flowfield and the soot model is achieved through a flamelet library approach, with transport of the moments of the soot particle size distribution function as outlined by Wenzel et al. [3]. In this work we extended this approach by considering acetylene feedback between the soot model and the combustion model. The model was further improved by using new gas-phase kinetics and new fitting procedures for the flamelet soot library. We investigated typical part-load operating points and a good agreement with the experimental data for soot in the exhaust gas was achieved when accounting for acetylene feedback.

INTRODUCTION

Because of its fuel efficiency the diesel engine is a very attractive power unit not only for medium and heavy duty vehicles, but also for passenger cars. However, it has also disadvantages compared to gasoline engines, in

particular with respect to soot and NO_x emissions. The increasing environmental pollution through vehicles powered by internal combustion engines induces worldwide the introduction of severe emission norms, as shown on the example of the EU legislative regulation in fig. 1. The EU6 norm valid from 2014 requires a reduction of the NO_x emissions down to 80 mg/km compared to 250 mg/km in the current EU4 norm.

As NO_x aftertreatment systems are expensive, the automobile manufacturers have reacted to those restrictions by developing new engine technologies aiming to reduce the raw NO_x emissions. The most effective one is the exhaust gas recirculation as it reduces the combustion temperatures and consequently the NO_x formation. However, it deteriorates the oxygen concentration and has thus a negative effect on the soot emissions. Consequently, the combustion chamber design and the interaction between spray and piston geometry have to be further optimized, so that a better air utilization and respectively lower raw soot emissions can be achieved.

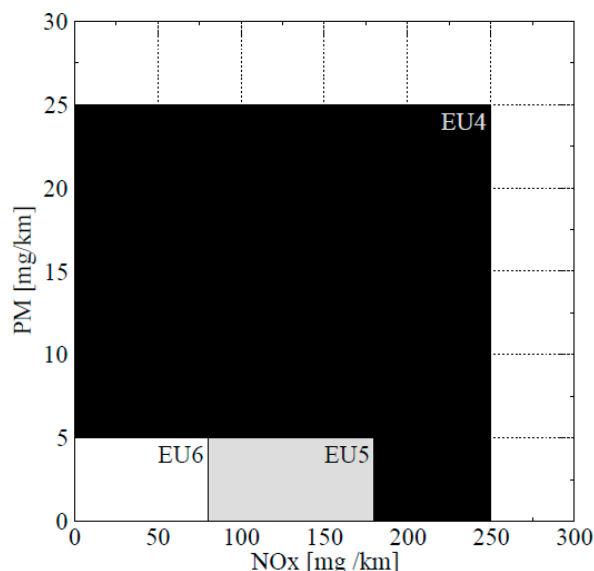


Figure 1: Emission standards for passenger cars in Europe [4]

The diversity of design parameters to be optimized poses challenges to the classical, experiment driven product development process. This makes CFD simulation attractive, in particular if it allows engine optimization at reasonable CPU time costs. CFD simulation is a valuable development tool especially in the case of investigating soot formation and oxidation, which are determined by local chemical and physical processes.

A major goal of the soot modeling work presented here is to develop a numerical tool capable of suggesting improvements to the combustion chamber design with respect of soot emissions. In this work, we describe the further development of the soot model presented in [3]. This paper is outlined as follows: First, the details of the soot model and its coupling to the turbulent flowfield are discussed. Next, the spray and combustion models are briefly described, followed by a description of the experimental validation cases and the computational setup. Finally a presentation of the results and conclusions are offered.

SOOT MODELING

REQUIREMENT SPECIFICATION

A detailed soot model for diesel engines includes a chemical model and a model for flow chemistry interaction. The requirements concerning a soot model as an integrated part of a 3D CFD simulation package for current and future combustion chamber design are as follows:

- The model should be generally valid for different engines and different engine operating regimes.
- The model should be capable of delivering local rates of soot formation and oxidation depending on

temperature and species concentrations within the computational cell.

- Effects associated with the detailed soot or gas phase chemistry should be realistically predicted without evaluating the detailed gas phase chemistry for the whole flow field.

The soot model should allow engine optimization within a reasonable computational time frame, which implies the introduction of a limited number of additional variables and equations to solve.

BACKGROUND SOOT MODELING

The formation of soot is one of the most complex chemical processes during the combustion of hydrocarbons. Soot particles containing more than 100000 carbon atoms are formed from simple hydrocarbons within a few milliseconds. Within the same time a large number of these particles are oxidized. The latter makes the prediction of soot emissions more difficult than the prediction of NO emissions. The process of soot formation is much more sensitive to flame temperature, radical levels etc. than other combustion processes. This justifies the demand on the accuracy of the chemical modeling.

Chemical models of any detail can be applied when studying simple laminar flame or reactor configurations. Keeping the accuracy of the chemistry submodel becomes a challenge when the complexity of the modeled configuration increases, i.e. when moving from simple laboratory configurations to real-world applications. A variety of models ranging from simple, parameter based models to detailed kinetic models have been proposed in the past for modeling soot formation in diesel engines. One of the most well known simple models, available in most commercial fluid dynamics software, is the Hiroyasu model [5] combined with the Nagle-Strickland-Constable oxidation model [6]. Although computationally efficient, such models rely heavily on user-tuning, which restricts general applicability. For diesel engine CFD applications, phenomenological models, such as the model by Hong et al. [7], have also been proposed. These models are often coupled with eddy-dissipation concept based combustion models and feature a global step reaction for building the first soot particle directly through acetylene. It has recently been shown that, even when using a simple soot model, the choice of how to select the species for particle inception will affect the CFD predicted soot lift-off location, as discussed by Vishwanathan et al. [8]. This motivates the need to use detailed PAH formation kinetics in a soot model applicable to a wide range of diesel engine operating conditions. Detailed gas phase and PAH formation kinetics can be handled in industrial product development CFD calculations through the use of an interactive flamelet model. Balthasar et al. [9] give a thorough discussion on the aspects of soot modeling

within the interactive flamelet framework, with specific emphasis on heavy-duty diesel engine development.

A recent study on the processes of soot formation and transport in reacting flows by the help of 3D DNS [10] showed that curvature effects can not be neglected. This questions if the inclusion of the soot transport in the interactive flamelet calculation is accurate enough for technical applications. In reference [11] rates of soot formation and consumption have been calculated from laminar flamelets and stored in a library of source terms for soot formation. Soot transport was calculated by the CFD code which accessed the flamelet library of sources. This method is further developed in this paper. An alternative to it is calculating the soot source term in the interactive flamelet, and calculating the transport equations in the CFD code. This approach includes transient effects – caused by rapid changes in scalar dissipation – on the rates of soot formation [12].

GENERAL CONCEPT

The idea implemented in the present study is to put most of the computational effort into the fluid dynamics using a relatively simple combustion model. Since soot formation is assumed to occur at time scales that are much larger than the turbulent time scales of the flow field, the soot formation and oxidation rates rather than soot mass fraction itself can be stored in the flamelet library [11,13,14]. The soot formation is described by a detailed kinetic model. The stored rates are divided into the rates of particle inception, surface growth, fragmentation, and oxidation by OH and O₂. These rates were precalculated in flamelet calculations and stored in flamelet libraries. In the next step the soot formation and oxidation rates were modeled as mathematical functions depending on a limited number of variables, which considerably reduces the size of the soot library. For accurate soot modeling it is also necessary to obtain the particle size distribution function (PSDF) of the soot particles. Since solving the PSDF is CPU time intensive the method of moments introduced by Frenklach [3,15,16] is applied. In the approach used here, source terms to the moments of the soot PSDF are partially evaluated through the use of a flamelet library. In the following we outline the basics of the detailed kinetic soot model and its coupling to a CFD code.

THE DETAILED KINETIC SOOT MODEL

The soot model used in this work is the detailed kinetic soot model described by Mauss [2]. The description of the different processes occurring in the gas phase and on the surface of the soot particles is based on detailed chemical and physical models. The soot model can be subdivided into three different parts (see Fig. 2):

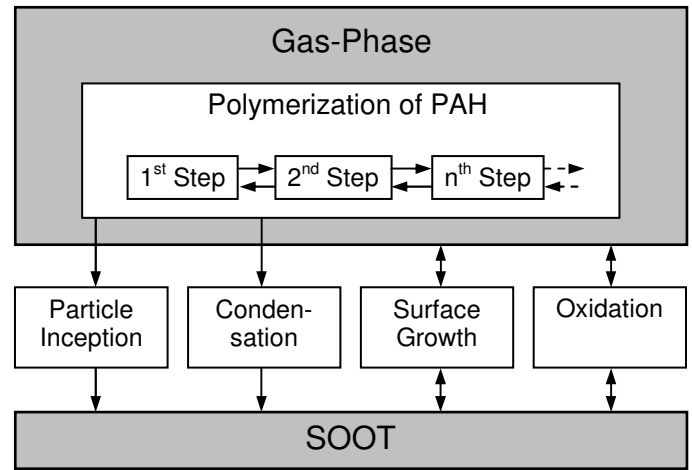


Figure 2: Illustration of the different soot processes

- Chemical reactions in the gas phase leading to the first small polycyclic aromatic hydrocarbons (PAH);
- Growth of the PAHs;
- Surface processes involving soot particles like particle inception, surface growth, fragmentation, and oxidation.

The modeling approaches applied will be described briefly in the following. A more detailed description can be found in [2,17].

MODELING OF THE GAS-PHASE CHEMISTRY AND PAH GROWTH

In earlier publications reaction mechanism for a mixture of n-decane and α -methyl-naphthalene as Diesel reference fuel was deployed [3]. In this work the chemical reactions in the gas phase are described by a detailed reaction mechanism for the combustion of n-heptane containing 121 species and 973 reactions [18]. The mechanism was extensively validated for numerous operating conditions [19]. The n-heptane chemistry was coupled with PAH (Polycyclic Aromatic Hydrocarbons) chemistry including pathways to benzene and further pathways describing the formation of the first small PAH, a species containing 24 carbon atoms (12 C₂ groups). This species represents the interface between the gas phase mechanism and the further growth of the PAHs. The PAH molecule grows in a repeating cycle of H-radical abstraction and addition of acetylene [20]. After the addition of two acetylene molecules a ring closure takes place and a new six-membered aromatic ring is added. This process repeats forming large PAHs that can coagulate and form the first soot particles (see Fig. 2). The growth of the PAHs is modeled as a fast polymerization process [2]. The underlying assumption is that the PAH reactions are fast or in other words that the formation of soot from the PAH is fast, so that the PAH molecules can thus be assumed to be in steady state. This results in a system of algebraic equations for the concentrations of the PAHs.

SOOT – GAS PHASE INTERACTION

Coagulation of two PAHs leads to the formation of the first soot particles. These particles can grow further by heterogeneous reactions of gas phase species with radical sites on the surface of the soot particles. The surface growth process is similar to the growth of the PAHs. The first step is an abstraction of a hydrogen radical from the soot surface, which is followed by an addition of C_2H_2 (HACA-mechanism, hydrogen-abstraction-acetylene-addition [20]). This process is assumed to be reversible with the reverse process leading to a fragmentation of acetylene from the soot surface at high temperatures [2,21]. The soot particles can grow due to condensation of PAH molecules onto the soot surface as well. The soot oxidation takes place on the particle surface by heterogeneous reactions of soot with molecular oxygen and hydroxyl radicals. The coagulation processes are described by the Smoluchowski equation [22].

As stated above, in the current work the method of moments introduced by Frenklach [15,16] is applied. The method is based on the fact that solving an infinite number of moments is equivalent to solving the PSDF itself and the assumption that the consideration of just some moments is sufficient to obtain good results in most applications. The moments of the PSDF are given by:

$$M_r = \sum_{i=1}^{\infty} i^r N_i; \quad r = 0, 1, \dots, \infty. \quad (1)$$

In the current study the number of moments was reduced to four:

- M_0 : Soot particles total number density
- M_1 : Soot volume fraction
- M_2 : Variance
- M_3 : Skewness

The method of moments is discussed further in ref. [23].

FLAMELET MODEL

The soot model described above can be applied to 1D laminar flame calculations. In the simulation of internal combustion engines a turbulent multidimensional reactive flow has to be taken into account. Hence, the soot model needs to be coupled to the turbulent flow field. The laminar flamelet approach developed by Peters [24] is applied in this study and described briefly in the following.

The basic idea of the flamelet approach is to decouple the chemical reactions from the turbulent flow field based on an analysis of the corresponding time scales. The coupling function hereby is the so called mixture

fraction. Under the assumption that the chemical reactions are fast compared to the turbulent time scales and occur in a thin reaction zone all species mass fractions are solely a function of this coupling function and the scalar dissipation rate χ . The turbulent flame can thus be regarded as an ensemble of laminar flamelets. The scalar dissipation rate χ represents the strain that the flow field introduces to the laminar flamelets.

A one-dimensional transport equation for the enthalpy, expressed in temperature and the species mass fractions is solved a priori to the flow field calculations. The stationary flamelet equations for temperature and species mass fractions by assuming equal diffusivities and a unity Lewis number of 1 can be written as:

$$\rho \frac{\chi}{2} \frac{\partial}{\partial Z} \left(c_p \frac{\partial T}{\partial Z} \right) + \rho \frac{\chi}{2} \sum_{i=1}^n c_{p,i} \frac{\partial Y_i}{\partial Z} \frac{\partial T}{\partial Z} = \sum_{i=1}^n h_i \dot{w}_i + \dot{q}_R \quad (2)$$

$$\rho \frac{\chi}{2} \frac{\partial^2 Y_i}{\partial Z^2} = -\dot{w}_i \quad (3)$$

$$\tilde{\chi} = c_{\chi} \frac{\tilde{\epsilon}}{\tilde{k}} \tilde{Z}^2 \quad (4)$$

In the classic flamelet library approach, the mass fractions and temperature are stored in the mixture fraction/scalar dissipation rate space into so-called flamelet libraries. Transport equations for the mean and the variance of the mixture fraction Z are solved and used to obtain the shape of the presumed PDF of mixture fraction. The mean mass fractions and temperature can then be obtained with the help of the PDF and the flamelet libraries. No transport equations for the species mass fractions have to be solved in the CFD code. But since soot formation is assumed to occur at time scales that are much larger than the turbulent time scales of the flow field the classical flamelet library approach as described above is not valid for the calculation of soot formation. In earlier works, e.g. [11,13,14,17] a transport equation for soot mass fraction Y_s was solved in the flow field and the rates of soot formation were precalculated in the flamelet calculations and stored in the flamelet libraries. In the approach used here, source terms to the moments of the soot PSDF are partially evaluated through the use of the flamelet library.

LIBRARY APPROACH

Flamelet libraries containing the rates of soot formation and oxidation have been calculated for a wide range of scalar dissipation rate, temperature on the flamelet oxidizer side, pressure and rate of exhaust gas recirculation (see Table 1). This wide range of boundary conditions was chosen to make the library applicable to simulation of soot formation in modern diesel engines.

Composition fuel	100% N-C ₇ H ₁₆
Composition air (by vol.)	79% N ₂ , 21% O ₂
Composition exhaust gas (by vol.)	12.4% CO ₂ , 14.2% H ₂ O, 73.4% N ₂
Temperature fuel side	350 K
Temperature oxidizer side	T = 250 – 1600 K
EGR range (containing only N ₂ , CO ₂ and H ₂ O)	EGR = 0 – 50%
Pressure	P = 1 – 250 bar
Scalar dissipation rate	χ = 0.05 – extinction limit

Table 1: Range of flamelet calculations

DARS [25] was used for the calculation of the flamelet libraries using an adaptive grid method in mixture fraction space to increase accuracy and a pseudo-arclength method automating the variation over scalar dissipation rate. A further simplification is required for practical use of the method in three-dimensional CFD simulations due to some restrictions:

- The library of soot formation and oxidation rates requires about 20 GB of memory space,
- An interpolation of the soot source terms from the library in five dimensions at every grid point is very time-consuming,
- A numerical integration of the laminar source terms over the mixture fraction and the scalar dissipation rate for turbulent averaging is also very time-consuming.

The flamelet libraries are therefore expressed in a simple analytical functional form. The beta-function was found to be a very good choice for modeling the dependence of the source terms on mixture fraction. The accuracy of this approach was nevertheless limited [26]. For this paper a double-beta function has been introduced that offers higher accuracy at the same computational costs. Figure 3 depicts the typical shape of the particle inception source term, and approximations with both single and double beta functions. As can be seen the accuracy of the approximation was improved by using two beta functions instead of one beta function.

The source terms as a function of mixture fraction Z are first normalized to have an area of unity. The approximation with double beta-functions is then done in two steps. In the first step one beta function is used to approximate the lean side of the source term. In the second step the second beta function approximates the difference between the original source term and the approximation with the first beta function.

For final usage of the library a method was developed to approximate the coefficients of the double beta function as function of the remaining library parameter; pressure, EGR amount, oxidizer side temperature, and scalar dissipation. The coefficients of the two beta functions are

interpolated in scalar dissipation and EGR, while a approximation with twelve suitably chosen functions is used to get the variation with oxidizer temperature and pressure. Figures 4a and 4b illustrate an example of the decrease of the mean relative error of the double beta procedure compared to the single beta procedure.

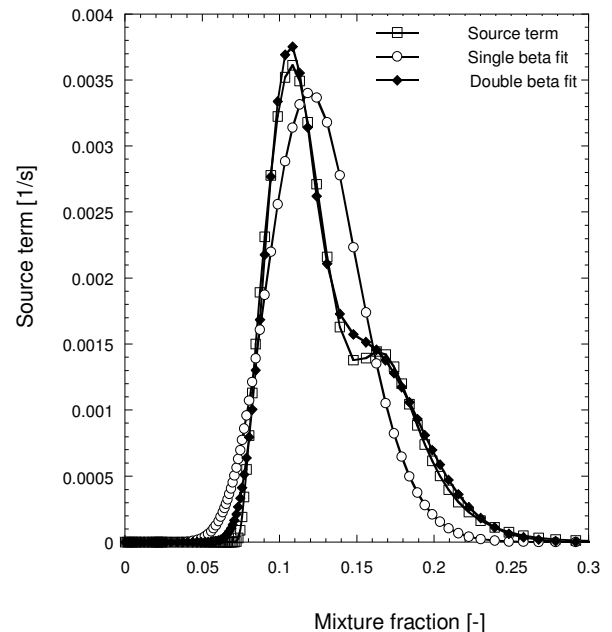


Figure 3: Sample particle inception source term, approximated with a single and a double beta function.

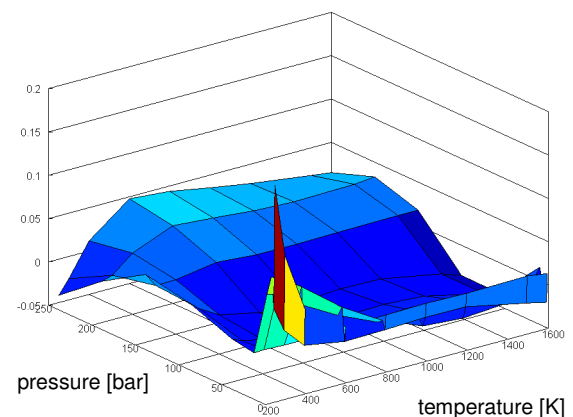


Figure 4a: Decrease of mean absolute error due to fit with double beta-functions compared to fit with a single beta-function (particle inception, EGR 0% and scalar dissipation rate 10s^{-1}).