Progress in Soot Modeling for Engines

R. R. Maly, P. Stapf and G. König

Daimler-Benz AG
Thermo- and Fluid Dynamics, FTI/T
D-70546 Stuttgart, HPC G206
Germany

ABSTRACT

A recent soot formation model using detailed chemistry was modified for high pressure applications. Since the required computing times do not allow a direct implementation in engine codes, the soot model was incorporated into a dedicated group combustion model to assess its performance under high pressure conditions. The combined model is capable of mimicking the microscopic details of combustion and pollutant formation in Diesel engines.

The model is based on a single droplet approach chosen to be characteristic and representative for the Diesel spray under consideration. The single droplet is exposed to the representative flow and combustion conditions of the engine. Using detailed chemistry and engine physics the full cycle of heating, evaporation, mixing, ignition, combustion and formation/depletion of NO and soot of the droplet are calculated. Sub-models for soot formation and oxidation by O₂ and OH account for a realistic description of the whole soot history. An extension of the NO chemistry accounts for prompt and thermal NO formation.

The model results are presented and discussed in view of available data showing good general predictive characteristics. Since the one-droplet model provides NO and soot data simultaneously it is regarded to be a very useful tool for guiding R&D work at reasonable computing expenses.

INTRODUCTION

Since practical exhaust aftertreatment systems for Diesel engines are still lacking, R&D efforts focus on the further optimization of the combustion process itself to simultaneously reduce pollutants and fuel consumption. To guide this work there is an increasing demand for predictive simulation tools to support the practical research and development efforts. If reliable soot predictions are to be made the whole Diesel combustion process must be calculable with reasonable accuracy requiring detailed fluid dynamics as well as detailed chemistry. Whereas the computation of NO-emissions is reasonably well understood there is still a significant lag in the modeling of soot formation and soot burn-out. In addition, current 3D-CFD codes for Diesel engines are still in a developmental stage requiring appreciable further efforts in the modeling of sprays and spray combustion before a truly predictive performance can be expected. In consequence, tuned phenomenological codes are used in parallel to the development of detailed codes to provide more accuracy (within a limited range of application) and reduced computing times. Therefore, a number of different modeling approaches are emerging in the literature trying to provide reasonable accuracy at affordable time expenses by simplifying either the fluid dynamics or the chemistry or both.

Based on recent advances in detailed soot [1,2] and droplet [3,4,5] modeling a single droplet model has been developed which offers a detailed insight into the current state of the art in soot modeling for engine conditions. The model and its results are discussed in view of soot data obtained in an optical Diesel engine. The model is also used to put simplified phenomenological models into perspective.

GENERALIZED SOOT MODEL

The generalized soot model discussed below is based on contributions by Frenklach et al. [6, 7], Prasinsis, [8], Mauß [2, 9], Lindstedt [10] and our own. Since our work follows in major parts the comprehensive and most recent work of Mauß [2] the various processes in soot formation and oxidation are only briefly touched upon here to put our modeling work into perspective. In the interest of easing general understanding graphical representations of the processes are preferred over equations whenever possible.

The different building blocks of our detailed soot model are presented in Fig. 1 and will be discussed subsequently in some detail. They center around a diffusion flame whose gas phase reactions are handled by the CHEMKIN [11] and a Heptane code [2, 12, 13], respectively.

Diffusion Flame Chemistry

A sufficiently detailed and accurate reaction kinetic model for treating the complex hydrocarbon chemistry of flames is the starting base for the detailed soot model. As improved mechanisms - especially for high pressure regimes [e.g. 14] - become available they can easily be integrated into the scheme. Since Acetylene plays a key role in soot forma-
tion its accurate prediction is important for the quality of the model. The mechanism includes therefore Benzene and higher PAH formation [12,16] to account for the generation of the appropriate gas phase composition needed for the subsequent soot formation processes. The detailed chemistry provides all species required for NO and soot production.

### Fig. 1 Building blocks of the generalized soot model.

**Formation of the 1st Ring**

The initial step in soot formation is the built-up of the first aromatic ring. The process is visualized in Fig. 2 showing a low and a high temperature route. Although the alternative route via a self-reaction of C₆H₆ is controversially discussed in the literature [9], it is also included into the mechanism:

\[
C₆H₆ + C₃H₃ \leftrightarrow C₃H₃ + C₆H₆
\]

The addition of H and the abstraction of H₂ followed by the addition of C₂H₂ are characteristic sequences driving all subsequent steps as it will become obvious in the following processes.

**Fast Polymerization**

After the initial formation of single aromatic rings larger PAHs are built by combination as shown in Fig. 3. The HACA reaction sequence - H-Abstraction, C₂H₂-Addition - first activates an aromatic molecule and adds then two more carbon atoms which in the case shown closes a third ring.

Hence by combination of aromatic rings and the HACA sequence a fast PAH growth process is started producing increasingly larger PAHs.

**PAH growth by the HACA Sequence**

Another route to initial PAH growth is shown in Fig. 4 demonstrating the sequential steps of aromatic activation, acetylene addition, H-abstraction and finally ring closure in detail. Depending on the site at which activation takes place different aromatic structures will be obtained as indicated schematically. During these early stages of PAH growth preferentially planar structures are formed. Since some aromatic species are particularly stable their reverse reactions are small and they will accumulate rapidly. The repetition of the sequence shown for 1-3 rings leads to ever higher PAH molecules. This might wrongly suggest that only growth processes will take place which, however, is not the case. Simultaneously with formation competing oxidation processes are also active in parallel reducing the size of the PAHs (see below).

**Aromatic Combination**

PAH growth beyond 4 aromatic rings is based on the linear lumping technique of Frenklach [6] visualized in Fig. 5. Again the growth mechanism is based on the HACA sequence. However, due to the additional incorporation of OH and O reactions as well as explicit reverse reactions a consistent formation and burn-out process for PAHs is established. Within each 5 step sequence 2 aromatic rings may be either added or removed. The computational advantage using a fast polymerisation process [2], based on a steady-state assumption for the PAHs, is that only a small number of differential equations is required to describe an infinite growth sequence. During the growth process hydrogen sites
are successively replaced by carbon atoms producing PAHs with an expanding inner carbon core and a hydrogen periphery.

Fig. 5 The linear lumping scheme used for the fast polymerization of higher order PAHs [6].

Oxidation

To limit the PAH growth process and to take care of lean burning conditions also, oxidation by OH and O₂ is included in the lumping sequence as shown in Fig. 6. Since the activation energy of OH is only 2/3 the activation energy of O₂ the OH is a much more efficient oxidizing agent than O₂. This is important for soot reduction in real engines where OH may be deficient at late crank angles. The scheme shows that 2, corresponding to 6 carbon atoms, will be removed by OH or O₂ in only 3 steps. It is also important to note that the oxidation products of the PAHs are not CO₂ but CO and hydrocarbon radicals, respectively.

Fig. 6 Oxidation of PAH by OH and O₂ [9].

Nucleation

The fast PAH polymerization continues until planar aromatic structures of about 80 carbon atoms have been formed corresponding to 12-14 aromatic rings. At that stage coagulation of PAHs occurs transforming 2 PAHs into 1 incipient soot particle with a mass of about 2000 amu. Due to coagulation the number density of the PAHs, and later in the process also of the soot particles, is reduced though mass and volume of the total soot remain the same. From now on we have 3-dimensional soot particles which may grow or shrink depending on surface reactions. The particle growth may be due to adsorption/condensation of PAHs on the surface or by coagulation of particles. For convenience in computation the particles are assumed to be spherical although experimental evidence shows open branched clusters.

\[
\text{Nucleation} \quad \text{PAH}_{2D,m} + \text{PAH}_{2D,n} \rightarrow \text{PAH}_{3D,m+n} = C_{\text{soot},m+n}
\]

\[
\text{Condensation} \quad C_{\text{soot},i} + \text{PAH}_{2D,n} \rightarrow C_{\text{soot},i+n}
\]

\[
\text{Coagulation} \quad C_{\text{soot},i} + C_{\text{soot},j} \rightarrow C_{\text{soot},i+j}
\]

\[\text{Number of Carbon Atoms} \quad \leftrightarrow \quad i, j, n\]

Fig. 7 Formation of 3-dimensional PAHs, e.g., particles, by coagulation of planar PAHs [2].

Soot Surface Growth

The surface growth process is treated in a similar way as in the HACA sequence. However, in contrast to PAH polymerization it is assumed here that the ring closure \((i \rightarrow i + 2)\) is irreversible [2] to allow the important surface growth at higher flame temperatures (Fig. 8). As will be shown later, soot growth and soot burn-out are now reasonably well determined by the mixture conditions and the flame temperature without a need for arbitrary tuning coefficients.

\[
\text{Growth:} \quad C_{\text{soot},i} + H \leftrightarrow C_{\text{soot},i} + H_2
\]

\[
C_{\text{soot},i} + \text{OH} \leftrightarrow C_{\text{soot},i} + H_2O
\]

\[
C_{\text{soot},i} + H \leftrightarrow C_{\text{soot},i}H
\]

\[
C_{\text{soot},i} + C_2H_2 \leftrightarrow C_{\text{soot},i}C_2H_2
\]

\[
C_{\text{soot},i}C_2H_2 \rightarrow C_{\text{soot},i+2}H + H
\]

\[
\text{Oxidation:} \quad C_{\text{soot},i} \rightarrow C_{\text{soot},i} + 2 + 2CO
\]

\[
C_{\text{soot},i}C_2H_2 \rightarrow 2O \rightarrow C_{\text{soot},i} + 2 + 2CHO
\]

\[
C_{\text{soot},i}H + \text{OH} \rightarrow C_{\text{soot},i} + 2 + \text{CHO} + \text{CHO}
\]

Fig. 8 Soot surface growth and soot surface oxidation [2].

Soot Radiation

Since radiation losses, especially in highly sooting rich flames, may account for appreciable energy losses - up to 30% [17] - the energy losses and gains of the volume elements of a diffusion flame must be accounted for. As shown in Fig. 9 this is achieved in a simplified manner by calculating the volume specific local black body radiation of the dominant gas and soot concentrations. Following Bressloff [18] and Madej [2] the energy absorbed due to radiation from the surrounding volume is calculated by using mean values for soot volume fractions, absorption coefficients and distances. The
energy balance - received energy minus emitted energy - is used to calculate the actual, local flame temperature which is very important for predicting soot correctly.

Specific Emission

\[ q_e = 4 \alpha \cdot \sigma \cdot T^4 \]

\[ \alpha = \alpha_s \cdot f_s + \alpha_{CO_2} \cdot P_{CO_2} + \alpha_{H_2O} \cdot P_{H_2O} \]

\[ \sigma = 5.669 \cdot 10^{-10} \text{W/m}^2\text{K}^{-4} \]

\[ \alpha_s = -3.75 \cdot 10^3 + 1.735 \cdot 10^4 \frac{T}{T_0} \]

\[ \alpha_{CO_2} = 46.241 \cdot \exp(-8.888 \cdot 10^4 \cdot T/T_0) \]

\[ \alpha_{H_2O} = 22.6 \cdot \exp(-1.546 \cdot 10^3 \cdot T/T_0) \]

\[ f_s = \text{Soot Volume Fraction} \]

Specific Absorption

\[ q_{abs} = \sum_j \alpha_{abs,j} \cdot q_{abs,j} \]

\[ \alpha_{abs,j} = 1 - \left( \frac{7 \cdot f_s \cdot \Delta x_s \cdot T}{c_2} \right)^4 \]

\[ c_2 = 1.439 \text{ cmK} \]

Fig. 9 Soot and gas radiation [2].

---

Fig. 10 Comparison of soot model predictions to experimental data from a 12 kPa Acetylene / Argon / Oxygen Flame. Dots: experimental data, dashed line: without radiation sub-model, dotted line: without coagulation sub-model, full line: complete soot model [19].

Model Verification

The principles outlined so far have been tested extensively on many different flames [e.g. 1,2]. An example of such a comparison is shown in Fig. 10 for the sooting characteristics of a low pressure Acetylene flame [19]. Three different test runs are shown demonstrating the importance of including radiation and coagulation sub-models. The full model gave an excellent agreement with the experimental data. Based on this agreement one can judge the relative effect of the different processes on soot growth as described above (see Fig. 11). The most dominant effects have the surface processes: growth, fragmentation (break-off of a CnHm) and oxidation. The obvious reason is that the particle surface is large already and eases a fast growth process. This does not imply, however, that the other processes are less important, on the contrary, surface processes depend crucially on the underlying elementary processes right down to the gas phase chemistry.

Fig. 11 Contributions of sub-models to soot formation and oxidation for a 12 kPa Acetylene / Argon / Oxygen Flame [19]

The detailed soot model may thus be applied with confidence to the low pressure range: \( p \leq 1 \text{ bar} \). However since these pressures are too far away from Diesel engine conditions, rigid tests and adaptations were necessary to render the model applicable to the more relevant pressures range: 1 to 100 bar.

Extension to high pressures

Numerous test calculations using the low pressure Mauß model [2] for the high pressure regime 1 - 100 bar revealed that predicted soot volume densities were much to low. As experimental data base the results of Mützing, Feldermann and Heidemann [20-22] were used. The main reason was identified to be the basic assumption in the low pressure coagulation sub-model of Mauß that the soot particles behave as free molecules and coalesce in each collision (collision efficiency = 1) overemphasizing the coagulation process at higher pressures. Therefore, the approach of Pratsinis - treating the coagulation process as a transitional regime between molecular and continuum motion [8] - was adopted for the regime \( p \geq 10 \text{bar} \). In the intermediate regime \( 1 \leq p \leq 10 \text{bar} \) a linear interpolation between the Mauß and the Pratsinis model was used.

Since the tests suggested minimal coagulation to occur at \( p \geq 70 \) an additional pressure dependent scaling function \( 3^{19} \).
order polynomial) was introduced for the effective coagulation rates having the following properties:

\[
\begin{align*}
    f_{\text{coag}} &= 1.0 & \text{for} & \quad p \leq 10\text{bar} \\
    f_{\text{coag}} &= 0.8 & \text{for} & \quad p \leq 35\text{bar} \\
    f_{\text{coag}} &= 0.0 & \text{for} & \quad p \geq 70\text{bar}
\end{align*}
\]

Using this modified coagulation model, it was possible to match the available high pressure data [20-22] reasonably well. Figure 12 shows a comparison between these data and our own calculations. The agreement is quite good in the intermediate pressure range \(2 \leq p \leq 50\text{bar}\) where most of the soot burn-out in engines will occur. The offsets in the 1 and 70 bar regions are considered to be still acceptable for trend calculations as envisaged by our droplet model. They need attention, however, when developing the model further.

![Graph showing soot volume fraction over time](image)

**Fig. 12** Comparison of experimental data [20-22] to soot model predictions for high pressures using the modified coagulation model.

**GROUP COMBUSTION MODEL**

To test the generalized soot model under conditions typical for Diesel engines, a group combustion model is used accounting in detail for the complex interactions between fluid dynamics, clusters of droplets and detailed combustion chemistry in sprays [4]. The concept of the model is shown schematically in Fig. 13. The abundance of droplets in a real spray is replaced by a small but representative droplet group (currently up to 20 droplets of different sizes). The flow field acting on the droplet group is replaced by a single, local, mean flow. Turbulent heat transfer to and evaporation of individual droplets are calculated using detailed physics.

![Diagram illustrating group combustion model](image)

**Fig. 13** Concept of the Group combustion model [4].

![3D temperature distribution](image)

**Fig. 14** Calculated 3D temperature distribution within a group of 10 Heptane droplets (6 x 15, 3 x 20 and 30 \(\mu\text{m}\)) at 0, 0.2, 0.3 and 0.4 ms after injection. Initial droplet velocity: 5 m/s right to left, incoming gas flow: 1.25 m/s left to right [4].

General transport equations are used for both the liquid and the gas phase. The model is composed of 2 stages: stage A models the 2D group interactions with global chemistry, stage B the detailed chemical processes in a 1D configuration around an individual droplet with the proper initial fluid and thermodynamic conditions provided by stage A. A 3D Low Mach Number formulation of the Navier-Stokes equations in a control volume formulation is used to eliminate acoustic waves and time scales [23]. The chemical kinetics of the detailed Heptane mechanism have been extended to account...
for the NO production/depletion by prompt as well as thermal processes [24]. The kinetics are solved simultaneously with the general conservation equations. In Fig. 14 the results of an ignition study of a group of 10 differently sized Heptane droplets are shown. The Diesel-like conditions used in the computation were:

- initial gas temperature: 1000 K
- initial droplet temperature: 350 K
- initial pressure: 50 bar
- initial gas composition: $\phi = 0; \theta = 0.33$
- engine speed 1130 rpm.

Fig. 15 Calculated ignition process of a 25 $\mu$m Heptane droplet injected into engine conditions at 3° b TDC and $\phi=0$. One-droplet model [25].

It will be noted from Fig. 14 that the temperatures may vary over wide ranges depending both on time and location. Hence evaporation and combustion are depending heavily on the local conditions as well. Ignition starts in the wake of the cluster slightly on the lean side where evaporated fuel had the longest time to react. A close-up view on the temperature evolution around a single droplet - calculated by the stage B model - is given in Fig. 15, a species distribution for 2 different gas conditions - air and $\phi = 0.33$ - in Fig. 16.

DETAILED 1D NO AND SOOT DROPLET MODEL.

To assess the applicability of the generalized soot model to Diesel engine conditions, the soot model was implemented into the one droplet model. It is thus possible to study the NO and soot formation processes simultaneously under identical high pressure conditions. The structure of the extended 1D droplet model is shown in Fig. 17.

The generalized soot model described above was incorporated into the stage B Heptane droplet model. The detailed chemistry is now used for both NO and soot calculations.

Fig. 16 Species distribution around a burning 25 $\mu$m Heptane droplet at 4° a TDC. Injection at 3° b TDC. Full lines: combustion in air, dashed lines: combustion in $\phi = 0.33$ Heptane / air mixture [4].

To this end it was extended to include recent mechanisms for the formation of aromatics and NO (prompt and thermal [26]) as well as for Heptane. The mechanism provides also the species needed for soot formation.

Fig. 17 Structure of the 1D NO and soot droplet model.

In the following section examples of model predictions will be presented for typical Diesel engine conditions at half load as listed above. Although a single droplet model will be a long way from a full spray model it will nevertheless be attempted to compare the one droplet model predictions to measured soot concentrations in a transparent Diesel engine operated under realistic conditions.

The motivation is to check the fundamental principles in modeling soot formation for engines which should show up in global data, e.g. total soot concentrations, if conditions are chosen properly.
Fig. 18 Calculated distribution of soot related species around a 25 μm Heptane droplet in an oxygen deficient environment represented by a 1%O₂ / 11.9% CO₂ / 13.3% H₂O / 73.8%N₂ mixture (equiv. to rich conditions) at 25° a TDC.

\[ P = 50 \text{ bar, } T_0 = 2000 \text{ K.} \]

Fig. 19 Calculated effect of temperature variation on the soot yield of a 25 μm Heptane droplet in a 1%O₂ / 11.9% CO₂ / 13.3% H₂O / 73.8%N₂ mixture (equiv. to rich conditions).

\[ P = 50 \text{ bar.} \]

An overview on the spatial distribution of soot formation around a burning heptane droplet and on the effects of temperature, oxygen concentration and droplet size on the total soot produced in a 55° crank angle interval is shown in Figs. 18-21. Although the decrease in cylinder pressure during the expansion stroke has not yet been accounted for (the pressure has been kept constant so save computing time) the model predictions agree well with general expectations based on engine experiments. A few points are interesting to note:

* the soot mass peaks at 2,200 K. This is caused by a faster increase with temperature of the soot burn-out rates than of the soot formation rates. Although less soot is formed at lower temperatures an even lesser amount is burned up during the oxidation phase making low temperatures rather unattractive for low particle combustion schemes.

* fast soot burn-out requires relatively high oxygen concentrations at the droplet location. Low concentrations (< 1%) delay soot formation and burn-out significantly.

Fig. 20 Calculated effect of oxygen concentration on the soot yield of a 25 μm Heptane droplet in a N₂ / O₂ / H₂O / CO₂ mixture. P = 50 bar, \( T_0 = 2000 \text{ K.} \)

Fig. 21 Calculated effect of the droplet diameter on the soot yield of Heptane droplets in a 1%O₂ / 11.9% CO₂ / 13.3% H₂O / 73.8%N₂ mixture (equiv. to rich conditions).

\[ P = 50 \text{ bar, } T_0 = 2000 \text{ K.} \]
However, the most significant effect on soot production is caused by the droplet size itself. The smaller the size the faster and more complete is the burn-out even under adverse conditions (e.g. 2000 K and 1% oxygen). This compares very favorably with the well-known effect of increasing injection pressure - producing smaller droplets - on soot emissions from engines. The results also indicate that a few bigger droplets may dominate soot emission especially if injected late. They also explain the well known effect of high soot emission due to large fuel ligaments when needle closing is bad.

A more rigid test will be made by comparing soot predictions at BOI (beginning of injection) and EOI (end of injection) to measured engine data as well as by relating the soot peaks for 0 and 10% EGR, respectively. To this end 2D 2-colour measurements were performed in an optical Diesel engine using a filming technique. By evaluating all frames of the films detailed experimental data on soot temperature and soot concentration as function of crank angle were obtained. Examples of the 2D 2-colour technique are shown in Fig. 22, examples of evaluated soot temperatures and concentration data are presented in Figs. 23 and 24.

![Fig. 22 Soot temperature and soot concentration distributions as measured by the 2D 2-color filming method in a modern Diesel engine.](image)

![Fig. 23 Measured soot concentrations in a modern Diesel engine at half load and 0% or 10 % EGR, respectively.](image)

![Fig. 24 Measured soot temperatures in a modern Diesel engine at half load and 0% or 10 % EGR, respectively.](image)

To account for the strong effect of droplet size on soot production and for the presence of many different droplet sizes in real sprays the comparisons are made on the basis of a simulated integral soot yield generated by 7 different drop sizes (see Fig. 21). Since the SMD (Sauter Mean Diameter) of the experimental spray was 10 μm the drop sizes selected for the soot calculation by the one-droplet model were:

\[ d_{\text{drop}} = 5, 10, 15, 20, 25, 30 \text{ and } 40 \mu m. \]

For convenience in computation the reasonable size distribution function used in the KIVA code was chosen [26]:

\[ g(\tau) = \frac{\tau^3}{6 \tau^3} \exp(-\tau/\bar{\tau}); \quad \bar{\tau} = \frac{r_{\text{mean}}}{3} = \frac{\text{SMD}}{6}. \]
Figure 25 gives an overview on the weighting effect of different SMD values on the relative droplet numbers. The larger the SMD the higher the contribution of bigger drops.

![Figure 25](image)

**Fig. 25** Effect of SMD on droplet size distribution [26].

1. 0% EGR, BOI: $T_0 = 1000$ K, 21% O$_2$, 11.9%CO$_2$, 13.3%H$_2$O, 73.8%N$_2$
2. 0% EGR, EOI: $T_0 = 2100$ K, 0.1% O$_2$, 1.25%CO$_2$, 1.4%H$_2$O, 78.45%N$_2$
3. 10% EGR, BOI: $T_0 = 1000$ K, 18.9% O$_2$, 11.9%CO$_2$, 13.3%H$_2$O, 73.8%N$_2$
4. 10% EGR, EOI: $T_0 = 2050$ K, 0.09% O$_2$, 11.9%CO$_2$, 13.3%H$_2$O, 73.8%N$_2$

The rationale for this selection is that droplets injected at BOI see the initial oxygen fraction and the compression temperature whereas those at EOI see only the oxygen left over from combustion and the higher product temperatures. Therefore, agreement is to be expected with experimental data for the rising or falling slopes of soot curves, respectively. The results of these computations are compared to the measured soot concentrations of Fig. 23 reproduced in Figs. 26 and 27. In all cases one notices a surprisingly good general agreement:

a.) the rising slopes of the BOI predictions fall on the extrapolated experimental rising slopes, and the falling slopes of the EOI predictions match well with the falling slopes of the experimental data both in the 0 and 10% EGR case,

b.) the relation between measured and predicted soot peaks for 0 and 10% EGR agree well, too.

The intermediate range is not accessible by the current approach since new and old droplet histories merge and produce less well defined situations as those at the beginning and end of injection.

The integrated soot yield was calculated by multiplying the soot yields of the individual droplets by the appropriate weighting factors according to the distribution function. Summing up over all 7 droplets and normalizing gives the total calculated soot yield to compare the experiments with. These calculations were made for mixture and injection conditions assumed to be reasonable for 4 cases without any tuning of the soot model:

![Figure 26](image)

**Fig. 26** Calculated soot yield at early and late injection of a 10 µm SMD distribution of Heptane droplets into Diesel engine conditions. Cases 1, 2. Bold: measured engine data.

![Figure 27](image)

**Fig. 27** Calculated soot yield of early and late injection of a 10 µm SMD distribution of Heptane droplets into Diesel engine conditions. Cases 3, 4. Bold: measured engine data.
CONCLUSIONS

1. It is concluded from the good overall agreement between predictions and available experimental engine data that the generalized soot model is well suited for Diesel applications. Since computing times are still rather high - due to the use of detailed chemistry - engine applications will necessitate the use of reduced schemes. The current model may be used advantageously to guide this work.

2. The fundamental character of the one-droplet model proved to be a very versatile and useful feature to clarify physics and chemistry in sprays. It is a very useful tool too, for developing better and faster spray models.

ACKNOWLEDGMENTS

The authors gratefully acknowledge the contributions by and many fruitful discussions with F. Mauß, H. Bockhorn, J. Warnatz and H.A. Dwyer.

REFERENCES