Detailed soot emissions predictions from a thermodynamic diesel engine model

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Abstract
This paper describes detailed soot emissions predictions from a multi-step phenomenological soot model implemented within a thermodynamic multi-zone diesel engine model. The soot model offers detailed insight into the following physical and chemical processes relevant to soot formation; acetylene formation and oxidation, precursor formation and oxidation, soot particle inception, particle coagulation and growth, and soot oxidation. Results of experimental and modelled cylinder pressure and heat release are initially presented to validate the diesel engine model. These are followed by predictions of the temporal evolution of net soot production, acetylene and precursor species yields, and soot number density at one operating condition. There is good agreement for soot mass predictions between the experiment and model. The results show that the soot model is suitable for use with thermodynamic multi-zone diesel engine models.

Keywords: soot, diesel, modelling, phenomenological

Nomenclature

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
</tr>
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<tbody>
<tr>
<td>TDC</td>
<td>Top Dead Centre</td>
</tr>
<tr>
<td>CAD</td>
<td>Crank Angle Degree</td>
</tr>
<tr>
<td>T</td>
<td>Packet temperature (K)</td>
</tr>
<tr>
<td>Ysoot</td>
<td>Soot mass (kg)</td>
</tr>
<tr>
<td>N</td>
<td>Soot particle number (1/m^3)</td>
</tr>
<tr>
<td>N_A</td>
<td>Avogadro’s number</td>
</tr>
</tbody>
</table>

1 Introduction

This paper presents detailed results from a multi-step model for the prediction of soot emissions from a diesel engine operating on diesel fuel; the soot model is implemented within a multi-zone thermodynamic diesel engine model. Thermodynamic diesel models have traditionally used simple empirical soot models similar to that first proposed by [1] are widely used in phenomenological diesel engine modeling (eg. [2]). These models offer the advantages of simplicity and low computational cost but lack a detailed insight into the physical and chemical processes that characterise soot formation and oxidation.

Other researchers, such as [3], have attempted to provide more realistic multi-step phenomenological models of soot production and oxidation. These models typically include processes such as precursor formation, particle inception, surface growth and particle oxidation. Models of this type have typically been used in CFD diesel engine models to provide inputs into the soot model, thus requiring extensive computing resources. The advantage of these models over the simpler two-step models is the ability to include particle dynamics and predict particle sizes and number density [3].

The aim of the present work is to integrate a complex multi-step phenomenological soot model into a multi-zone thermodynamic diesel engine model previously described in [4]. Predictions of cylinder pressure and heat release are presented to validate the diesel engine model. This is followed by predictions of net soot emissions, acetylene and precursors production and soot particle number density.

2 Modelling

2.1 Thermodynamic diesel engine model
The underlying diesel engine model has been presented in detail in a previous paper [4]. A brief summary of equations used and approaches taken is provided in this section. The cylinder volume is divided into two zones - the burnt zone, containing the spray, entrained air and combustion products, and the unburnt zone, containing air. The spray is divided into packets in the axial and radial directions. A global cylinder temperature is determined from the burnt and unburnt zone temperatures and used to calculate cylinder pressure using the equation of state. Individual packet volumes are calculated and integrated over the burnt zone to give the total burnt zone volume.

Spray tip penetration and break-up equations were taken from [5]. A comprehensive sensitivity analysis of the diesel engine model to different step sizes and numbers of radial zones has been presented previously [4]; based on convergence of cylinder pressure

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predictions and computational time, a step size of 0.2 CAD and 10 radial zones was found to be sufficient to eliminate numerical sensitivity of the model. These values have not been changed for the present investigation. There are as many axial packets as there are computational steps during the injection process. Each packet contains the same mass of fuel but different masses of air and products. A description of the air entrainment model is given in the original paper [4]. Different packets experience their own individual delays. When the first packet starts to burn, all packets that have exceeded the spray break-up length are allowed to start burning. This is an approach also used by [6]. For these packets, combustion occurs in two distinct stages. Fuel that was injected during the ignition delay period burns at the premixed rate; when this reservoir of fuel is burnt, combustion is controlled by the mixing rate of air into individual packets. For packets that had not exceeded the break-up length when the first packet started to burn, only mixing-controlled combustion is allowed. The empirical Arrhenius correlations for both stages were taken from [5] and are given in the original paper [1].

Heat transfer was calculated using the model proposed by [7]. A large number of arbitrary constants require tuning for phenomenological diesel engine models to provide useful predictions. A comprehensive discussion of the calibration process followed here is provided in [4].

2.2 Soot modeling

The phenomenological soot model used here is based on the work of [3]. The rate constants used are given in Table 1; some values have been modified for better agreement with experimental results. The rate of acetylene formation is given by,

\[ \dot{R}_1 = \frac{m}{2} k_1 [Fuel] \]

where \( m \) is the number of carbon atoms in the fuel (\( m=14 \)) and \([\cdot] \) denotes molar concentration.

Precursor formation is given by,

\[ \dot{R}_2 = \frac{2}{z} k_2 [C_2H_2] \]

where \( z \) is the number of carbon atoms in the precursor species (\( z=60 \)).

The presence of precursors leads to the inception of particles, as given by,

\[ \dot{R}_3 = z k_3 [R] \]

The diameter of the incepted particles is assumed to be 1.28 nm. However, coagulation of particles leads to an increase in particle diameter. The rate of coagulation is given by,

\[ \dot{R}_4 = \frac{1}{2} k_4 N^2 \]

where \( N \) is the soot number density. The constant \( k_4 \) is the collision frequency constant and is calculated using the same method as that of [3].

The diameter of the particle at this stage is given by,

\[ d_p = \left( \frac{6 M_C y_{soot}}{\pi N \rho_{soot}} \right) \]

where \( M_C \) is the molecular weight of a carbon atom, \( \rho_{soot} \) is soot density and \( y_{soot} \) is the molar concentration of soot.

Acetylene is adsorbed onto the surface of soot particles at the rate given by,

\[ \dot{R}_5 = k_5 [C_2H_2] (A_{soot})^{1/2} \]

where \( A_{soot} \) is the total surface area of the soot particles.

The rate of oxidation is proportional to the net soot mass and is given by,

\[ \dot{R}_6 = k_6 m_{soot} \]

The OH radical can also contribute to soot oxidation; the rate of oxidation by OH is given by,

\[ \dot{R}_7 = k_7 m_{soot} \]

Finally, both acetylene and the precursor species are oxidised. The rate of acetylene oxidation is given by,

\[ \dot{R}_8 = k_8 [C_2H_2] [O_2] \]

Precursor species oxidation is given by,

\[ \dot{R}_9 = k_9 [R] [OH] \]

Net soot formation is given by,

\[ \frac{d}{dt} (N_{soot}) = M_C (\dot{R}_3 + \dot{R}_5 - \dot{R}_6 - \dot{R}_7) \]

Total particle number density is given by,

\[ \frac{d}{dt} \left( \frac{N}{N_A} \right) = \frac{M_C}{M_{N_{soot}}} (\dot{R}_3 - \dot{R}_4) \]
Table 1. Rate constants used

<table>
<thead>
<tr>
<th>Rate constant</th>
<th>Value</th>
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<tbody>
<tr>
<td>$k_1$</td>
<td>$1.0 \times 10^{10} \exp (-25000/T)$</td>
</tr>
<tr>
<td>$k_2$</td>
<td>$1.0 \times 10^{11} \exp (-20000/T)$</td>
</tr>
<tr>
<td>$k_3$</td>
<td>$5.0 \times 10^{10} \exp (-25200/T)$</td>
</tr>
<tr>
<td>$k_5$</td>
<td>$1.04 \times 10^4 \exp (-3100/T)$</td>
</tr>
<tr>
<td>$k_7$</td>
<td>$1.4 \times 10^{11} \exp (-25200/T)$</td>
</tr>
<tr>
<td>$k_8$</td>
<td>$6.0 \times 10^{18} \exp (-25200/T)$</td>
</tr>
<tr>
<td>$k_9$</td>
<td>$1.0 \times 10^{17} \exp (-25000/T)$</td>
</tr>
</tbody>
</table>

3 Experiments

Experiments were performed using commercial diesel fuel in a direct injection naturally aspirated 4 litre 4 cylinder Hino W04D engine without EGR coupled to a Heenan Froude eddy current dynamometer and Froude-Hofmann V4 dynamometer controller. The engine is fully instrumented to record engine and in-cylinder parameters; injection timing was unchanged for the duration of this study. Further engine specifications and details of the laboratory setup are given in [4]

A National Instruments 24bit 1 Hz analogue to digital converter was used to read performance data, and AVL piezoelectric high-pressure transducers and a needle lift indicator were fitted into cylinder 1 to record cylinder and fuel injection pressure and needle lift respectively. Temperatures were measured using thermocouples. Fuel consumption was measured using a sensitive mass balance. Soot measurements were taken by passing undiluted exhaust gas into a TSI DustTrak DRX8533 laser light scattering photometer; exhaust gas temperatures were less than 51ºC at the point of sampling. Soot measurement results were calibrated against a gravimetric method using Pallflex Fiberfilm T60A20 membrane filters.

4 Results and Discussion

Figure 1 and Figure 2 show modeled and experimental cylinder pressure predictions, and rate of heat release (ROHR) and cumulative heat release for 1600 RPM, 100 Nm respectively; a previous paper [4] contains further results for a wider range of operating conditions. ROHR has been normalised by the maximum value of the cumulative heat released for all cases. Ignition delay is generally well predicted. The premixed combustion peak is generally lower than the experimental premixed peak; however, there is good agreement between modelled and experimental cumulative heat release at the end of the premixed phase. The modelled ROHR curve shows twin peaks of premixed and diffusion-controlled burning that are characteristic of the method of modelling used, even though this sharp distinction is not seen in the experimental curves. The figures show that the model is generally able to provide good predictions of cylinder pressure and heat release for the wide range of conditions presented.

Figure 3 shows the temporal evolution of cylinder-average soot mass production for 1600 RPM, 100 Nm. There is good agreement for the final soot mass value between the experiment and the model. The bulk of soot production occurs in a short period around TDC, followed by a substantial period of oxidation. Although not presented here, the maximum experimental uncertainties over a range of engine loads were less than 2%.

Figure 4 shows the cylinder-average temporal evolution of acetylene yield and precursor species in moles. Similar to soot formation acetylene formation and precursor species production peaks around TDC; thereafter, they are rapidly consumed and oxidised. These results are in broad agreement with previous investigations using similar models [3].
Figure 3. Temporal evolution of soot production for 1600 RPM, 100 Nm.

Figure 5 shows the cylinder-average temporal evolution of soot number density for 1600 RPM, 100 Nm. The profile of the curve is similar to those presented earlier; there is an initial rapid rise in particle numbers around TDC but the number of particles decreases rapidly after this point. Net particle number density is given by the difference between particle inception and coagulation. Thus, inception is shown to dominate for the initial period, while coagulation is the dominant phenomenon after this initial rise.

5 Conclusions

This paper presents results from a complex multi-step phenomenological soot model integrated into a multi-zone thermodynamic diesel engine model. The model is able to predict the temporal evolution of net soot production, acetylene and precursor species and soot particle number. These results are similar to those presented elsewhere in the literature.

While simple semi-empirical soot models have hitherto commonly been used in thermodynamic diesel engine models, it is likely that models that provide more detailed insight will be required in the near future. Models similar to the one presented here have previously been adopted for CFD diesel engine modeling. Their use in thermodynamic models offers potential improvements over the ubiquitous two-step soot models commonly used. Given the many advantages of thermodynamic diesel models over complex CFD models, it is proposed that this model is suitable for offering a detailed insight into the physical and chemical processes relating to net soot production.

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