CFD Modelling of Soot Formation and Entrainment Processes in Diesel Engine Combustion of Soy, Palm and Coconut Methyl Esters

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Abstract. The aim of this work is to employ computational fluid dynamics (CFD) modelling to elucidate the soot formation and entrainment processes when diesel as well as soy, palm and coconut methyl esters (biodiesel) are used in a light-duty diesel engine under varying operating conditions. ANSYS FLUENT 13, which is linked to a chemical kinetic model via CHEMKIN-CFD, a plug-in chemistry solver, is utilised. The soot entrainment focuses on thermophoretic soot deposition on the cylinder liner and soot transport into the crevice region via blowby. During the closed cycle combustion process, the mass of soot deposited on liner via thermophoresis is more significant than that transported into the crevice region through blowby, representing at least 95% of the total soot entrained. The percentage of entrained soot from the net amount of exhaust soot is dependent on the methyl ester type. Diesel results in the maximum soot entrainment with the largest averaged diameter while coconut methyl esters with short hydrocarbon chain length produces the smallest amount and size of entrained soot. Different saturation levels give rise to different soot entrainment processes under varying operating conditions. Overall, this work provides detailed insights into the main in-cylinder processes controlling soot entrainment for biodiesels.

1. Introduction
Excessive soot concentration in diesel engine oil can clog filters and form carbon deposits, which result in oil starvation and engine damage. Wear happens if the anti-wear additives are adsorbed onto soot. Furthermore, the viscosity of the engine oil viscosity increases leading to more friction cum increased engine wear rate. The soot particles size is another factor with soot diameters approaching the oil film thickness accelerating the wear rate of the engine. High soot concentrations exceeding tenfold the exhaust soot concentrations are present in the diesel engine combustion chamber. The local temperatures very near the chamber wall (several hundred microns) are significantly lesser thereby here, the soot particles may not undergo oxidation. This temperature gradient leads to thermophoresis, a major soot deposition pathway on in-cylinder surfaces. The soot particles migrate to the region of decreased temperatures and are deposited onto the wall of the combustion chamber. These soot particles are entrained into engine oil during exhaust blowdown via the crevice and through crevice blowby.
Recent works have shed light on the soot formation and entrainment processes in diesel engines [1–4]. However, to the authors’ best knowledge, there have been no comprehensive numerical studies comparing the in-cylinder processes affecting soot entrainment for different methyl esters (biodiesel), specifically soy, palm and coconut methyl esters (SME, PME and CME). This work addresses this limitation by utilising computational fluid dynamics (CFD) modelling to ascertain the effects of biodiesel saturation level and hydrocarbon chain length on soot formation and entrainment.

2. Numerical formulation and setup
ANSYS FLUENT 12 plus the chemistry solver CHEMKIN is used for the computational mesh generation and CHEMKIN-CFD modelling. The diesel engine specifications and fuel physicochemical properties are reported in [1]. The fuel injection parameters for diesel, SME, PME and CME at engine powers of 0.5, 1.5 and 2.5 kW are listed in Table 1. Only the closed part of the engine cycle is simulated (intake valve closure at -140 crank angle degree (CAD) after top dead centre (ATDC) till exhaust valve opening (EVO) at +140 CAD ATDC). The computational mesh represents a symmetrical 90° sector of the combustion chamber since there are 4 injector nozzle holes which are spaced equally. The cell size of 1.5 mm results in grid independent results. In the region next to the liner which extends into the crevice volume, the mesh is further refined into 0.07 mm thickness to enhance the results resolution. A 0-D ring-flow crevice model is used to model the effect of crevice flow below the top ring since this takes into account the axial flow velocity near the piston head and the liner which impacts species transport and soot entrainment [5].

Table 2 summarises the models used in the computational study. Further details on the use of the models can be found in [1, 3]. SME and PME with similar hydrocarbon chain length are used to compare fuels with different saturation levels (90% and 50% unsaturated, respectively). CME is chosen to study the effect of short hydrocarbon chain length. A user-defined function which includes two user-defined scalar transport equations developed by [2] is implemented to determine the soot particle number and deposited liner soot mass. The source terms are dependent on the soot concentrations cum thermophoretic velocity. Solution of the equations is conducted for the neighbouring zone cells of the cylinder liner. In the soot model, the same source terms are added as minus values to the equations of transport to obtain the soot mass fraction and normalised radical nuclei concentration, which maintains the wall-deposited and in-cylinder soot conservation.

Table 1. Fuel injection parameters (pressure=210 bar and coefficient of discharge=0.75).

| Power | SOI (CAD ATDC) | EOI (CAD ATDC) | Fuel consumption (kg/hr) | Total injection quantity (mg/cycle) | Initial pressure (bar) | Initial temperature (K) |
|-------|----------------|----------------|--------------------------|-------------------------------------|------------------------|------------------------|
| 0.5 kW| -13.5          | -5.79          | 0.236                    | 3.93                                | 1.23                   | 313                    |
|       |                |                |                          |                                     |                        |                        |
| 1.5 kW| -13.5          | -0.37          | 0.402                    | 6.70                                | 1.27                   | 323                    |
|       |                |                |                          |                                     |                        |                        |
| 2.5 kW| -13.5          | 5.74           | 7.34                     | 13.5                                | 7.41                   |                        |

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Table 2. Models used in CFD modelling.

| Model                  | Type                                               |
|------------------------|----------------------------------------------------|
| Fuel spray             | Kelvin–Helmholtz/Rayleigh–Taylor                   |
| Discrete phase         | Wall-jet                                           |
| Turbulence             | Renormalisation Group (RNG) k-ε                    |
| Near-wall region       | Standard Wall Functions                           |
| Reaction mechanism     | n-heptane and combined biodiesel surrogate         |
| Soot formation         | Moss-Brookes                                       |
| Soot oxidation         | Fenimore-Jones                                     |

3. Results and discussion

3.1. Soot deposition into liner

Figure 1 compares the deposited liner soot mass to the total tailpipe soot mass while Table 3 lists the soot particle sizes. Generally, the fuel that produces the largest amount of exhaust soot results in the maximum soot deposition. As such, the use of SME increases the soot mass deposited on the liner as compared to PME at low and medium engine powers. At high engine power, the amount of deposited soot for PME increases to higher than that of SME. However, the deposited soot particle size produced by SME is comparatively smaller at low power and larger at high power in comparison to PME. CME fuel produces the smallest deposited liner soot amount and particle size while diesel produces both the largest soot amount and particle size. At medium and high engine powers, the difference in the soot deposited on the liner between the cases of diesel and methyl esters remains within 3 orders of magnitude while at low power, it is increased to 5 orders of magnitude. Figure 1 illustrates the percentage of the net soot deposited onto the liner and transported into the crevice region. The difference in the soot deposited on the liner between diesel and methyl esters is largest at low engine power at approximately 3 orders of magnitude higher for diesel. All methyl esters produce similar percentage of deposited soot at low engine power. At medium power, the percentage of deposited soot increases proportionally with the exhaust soot level, with CME being the lowest and diesel the highest. A change of trend is observed between PME and SME when the engine power is increased. At high engine power, PME results in a higher percentage of deposited soot on the liner despite its lower exhaust soot level.

Figure 2 are the images of predicted soot concentration as side view projections of the 3-D soot iso-surfaces with semi-transparent layers of soot cloud. In every case, the soot images are shown from +20 to +60 CAD after the start of injection (ASI) to allow soot propagation monitoring. The higher gas temperature of diesel combustion is most evident at low engine power. Furthermore, the formation of soot cloud expands outwards of the piston bowl to the swept volume only for diesel while the soot cloud produced by all methyl esters concentrates inside the piston bowl. This results from the shorter injection duration which limits the fuel spray penetration in addition to the lower equivalence ratio near the piston bowl rim produced by methyl esters. Hence, the soot deposition process as caused by the diffusion of soot cloud towards the liner occurs later for methyl esters. Figure 2 shows that the soot cloud occupies two regions for most cases especially at higher engine powers, which are inside the piston bowl and in the swept volume near the liner. At medium power, it is observed that the soot
cloud close to the liner for SME is larger than that of PME, although the soot clouds inside the piston bowl are of similar sizes.

As engine power increases to a high level, the amount of deposited soot in the PME case increases to higher than that of SME. The combustion of PME improves at high engine power as its surface tension reduces with increased temperature thereby promoting evaporation. Hence, the in-cylinder temperature and the temperature gradient at the liner increase. Although the high temperature near the liner contributes to increased deposition rate, it also leads to high soot oxidation rate. The oxidation process of the soot particles results in smaller diameter prior to the deposition process. Conversely, the soot particle size in the SME case is smaller at low power. SME fuel has a higher combustion efficiency at low power due to the absence of the mixing-controlled combustion phase and its high initial evaporation rate. This is reflected in the higher in-cylinder temperature especially near the liner as highlighted in Figure 2. The high temperature increases the soot oxidation rate faster than its formation rate. With improved combustion and soot oxidation, the soot particles size is reduced.

Other than low exhaust soot, CME fuel produces the smallest percentage of soot deposited on the liner with the smallest diameter. It is observed from Figure 2 that the maximum local gas temperature is the lowest when CME fuel is employed. Due to its low equivalence ratio, the lean combustible mixture is spread to a wider region. Regardless of the similar distance of the combustion region from the liner, the temperature gradient is greatly reduced. With the lowest soot concentration and the combustion being overall lean as compared to other fuels, a high level of oxidation results in the smallest soot particle.

3.2. Soot transport into crevice

In all test cases, a higher amount of net soot produced in the combustion chamber results in a higher amount of crevice soot. From Figure 1, at low power, diesel produces the highest percentage of crevice soot while methyl esters exhibit similar levels. The highest percentage of soot in crevice results from diesel at medium power, followed by SME, PME and CME. As engine power increases to a high level, the trend changes for the results of diesel and CME. Diesel produces the lowest percentage of crevice soot regardless of the high exhaust soot level while CME has the highest percentage of soot in crevice. This is linked to the difference between the soot clouds in the piston bowl produced by the two fuels becoming more evident as the amount of fuel delivered is increased. Soot formed inside the piston bowl has a larger impact on the soot transport into the crevice than soot deposition on the liner as it propagates towards the crevice along the piston top. Observing the soot cloud at +60 CAD in Figure 2, the region of high soot concentration is located nearer to the centre of the combustion chamber for diesel. The high evaporation rate of diesel results in a high equivalence ratio of the spray core which extends towards the injector thus resulting in a high soot concentration near that region. In contrast, the soot produced by CME combustion has higher concentration around the piston bowl rim, which is nearer to the crevice. Due to the lean nature of the CME fuel spray, soot formation is higher at the bowl rim as the fuel impingement increases the equivalence ratio near the surface.

Across the tested engine powers, soot in crevice accounts for the highest percentage from the total soot entrained at low engine power (2–4%). The ratio of the amount of soot transported into crevice to the soot deposited on the liner drops as engine power increases. At high power, the increasing amount of soot results in a larger surface area of soot deposition site on the liner hence the amount of soot in the crevice becomes less significant comparably.

3.3. Total soot entrainment

Table 3 lists the total soot entrainment, which is the addition of the soot mass inside the crevice to the deposited liner soot mass. The latter is the major influencing factor in total soot entrainment as soot entrained into crevice accounts for less than 5% only of the total entrainment. Overall, the employment of methyl esters reduces the amount of soot entrained as compared to diesel in all cases. The difference in the outcome of soot deposited on the liner between diesel and methyl esters is largest.
at low engine power whereby the soot produced by methyl esters combustion is minimal. The effect of methyl esters physicochemical properties on the amount of soot entrained is also insignificant at low power. The saturation level instead has varying effects as engine power increases. At medium engine power, SME with a high unsaturation level produces a larger amount of soot entrained with smaller particle size as compared to that produced by PME. However, when engine power is high, the improved evaporation rate of PME at higher temperature enhances combustion and soot oxidation. The high combustion temperature gives rise to increased rate of soot entrainment, regardless of the lower net soot level in the combustion chamber. It is also deduced that the effect of temperature gradient on the thermophoretic deposition is greater at high engine power as the larger volume of combustion region brings the high temperature region closer to the liner. Contrastingly, CME with a shorter chain length reduces the soot entrained. With increased fuel bound oxygen content, the combustion of the lean fuel mixture reduces soot formation as well as combustion temperature, both of which affects the soot deposition process.

**Figure 1.** Mass of soot deposited on liner and total tailpipe soot (left; scaling factor for soot deposited on liner for diesel at 0.5 kW = 0.001) and percentage of soot deposited on liner and transported to crevice from net soot (right) for engine powers of (a) 0.5 kW, (b) 1.5 kW and (c) 2.5 kW.
Figure 2. (Left) Spatial evolution of soot and (right) temperature contour at the cross-sectional plane along the spray axis for engine powers of (a) 0.5 kW, (b) 1.5 kW and (c) 2.5 kW.
Table 3. Soot entrainment and particle sizes for varying fuel types and engine powers.

| Power | Fuel Type | Diesel | SME | PME | CME |
|-------|-----------|--------|-----|-----|-----|
| 0.5 kW | Total soot mass (x10^{-12} kg) | 51.2 | 9.88 | 9.78 | 0.01 |
|       | Soot mass in crevice (x10^{-22} kg) | 68.0 | 0.033 | 0.030 | 0.0005 |
|       | Soot mass deposited on liner (x10^{-21}kg) | 284.7 | 0.090 | 0.062 | 0.0021 |
|       | Total soot entrained (x10^{-21}kg) | 291.5 | 0.093 | 0.065 | 0.0021 |
|       | Entrained soot particle size (nm) | 1.345 | 0.084 | 0.092 | 0.046 |
| 1.5 kW | Total soot mass (x10^{-10}kg) | 54.5 | 14.2 | 8.9 | 0.65 |
|       | Soot mass in crevice (x10^{-19}kg) | 33.2 | 2.96 | 0.40 | 0.00 |
|       | Soot mass deposited on liner (x10^{-15}kg) | 41.2 | 7.17 | 1.13 | 0.01 |
|       | Total soot entrained (x10^{-15}kg) | 41.2 | 7.17 | 1.13 | 0.01 |
|       | Entrained soot particle size (nm) | 12.69 | 4.89 | 2.06 | 0.84 |
| 2.5 kW | Total soot mass (x10^{-8}kg) | 9.73 | 5.67 | 5.46 | 2.58 |
|       | Soot mass in crevice (x10^{-19}kg) | 51.5 | 31.2 | 22.4 | 0.22 |
|       | Soot mass deposited on liner (x10^{-13}kg) | 16.75 | 6.04 | 6.27 | 0.29 |
|       | Total soot entrained (x10^{-13}kg) | 16.75 | 6.04 | 6.27 | 0.29 |
|       | Entrained soot particle size (nm) | 22.73 | 9.32 | 6.63 | 5.48 |

4. Conclusions

Soot deposition on the liner is the major contributor of soot entrainment, representing at least 95% of the total soot entrained. Both the temporal cum spatial evolution of the soot cloud from the start of the soot deposition affect the process mainly through the dissimilarity of the air-fuel mixture equivalence ratio and the in-cylinder temperature which influences the wall temperature gradient. Diesel produces the largest soot entrainment (291.5x10^{-21}–16.75x10^{-13} kg) with the largest soot size (1.345–22.73 nm). CME with short hydrocarbon chain length produces the smallest entrainment (0.0021x10^{-22}–0.29x10^{-13} kg) and soot size (0.046-5.48 nm). Methyl esters with different saturation levels affects the soot entrainment process differently at varying engine powers. The deposited soot does not demonstrate similar proportionality to the amount of exhaust soot.

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