Coupling Effects of Chemical Kinetics and Start of Injection Strategies on Soot Emission in a Light-Duty Direct-Injection Diesel Engine

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Abstract. In this reported work, the numerical simulation of 3-D in-cylinder combustion and soot formation was carried out with ANSYS FLUENT 18.1 software. Here, two different combustion models (namely MCDS1 and MCDS2) were integrated to demonstrate the effects of aromatic components on soot formation. While both the surrogate models include straight- and branched-alkanes as its constituent hydrocarbon species, MCDS2 contains additional aromatic components to better represent the diesel fuel properties. Here, the start of injection timing was varied, i.e. at −6°, −2°, and +2° after the top dead centre, to study its effect on the soot emission performance after appropriate model validations. Clear reduction in soot yield was observed with advanced injection timing of −6° after top dead centre, in which the soot oxidation rate was found to be higher with earlier start of injection timing. This may be attributed to the higher in-cylinder temperature which enhances the soot oxidation rate. As compared to MCDS2, it was observed that the combustion of MCDS1 has consistently led to higher soot yield across all the cases. This can be attributed to its higher content of straight- and branched- alkanes.

1. Introduction

Due to the environmental impacts and harmful health effect caused by the pollutants in diesel exhaust gases, emission standards for diesel vehicles have become stricter to better regulate the air quality. To illustrate, chronic exposure to particulate matter (PM) from diesel exhaust has been linked with a series of diseases, in addition to premature death resulting from cardiopulmonary disease and lung cancer. As a result, reducing tailpipe soot emission remains to be the main objective in order to satisfy these emission target. With the introduction of electronic fuel injection system, the emission levels of diesel engine can now be controlled without compromise to engine performance. The modern common rail systems have enabled flexibility in injection timing which initiate a whole range of study into optimizing injection rate for engine performance and emission reduction. In general, advanced injection timing will likely result in reduced soot emission at the cost of higher NO\textsubscript{x} emission. Likewise, retarding injection timing causes reduced NO\textsubscript{x} emission at the cost of increased soot emission [1]. Nevertheless, injection timing should be fine-tuned for each engine and fuel configuration to achieve a balance between performance and emissions. Advancing beyond a certain limit may back fire and leads to poor performance and high smoke emission. By studying the relationship between fuel injection strategies and soot emission, this study may contribute towards the on-going research into cleaner engine technologies.

The study aims to investigate the relations between start of injection (SOI) timing and soot formation in direct-injection diesel engine with the use of two kinetic models with different fuel compositions,
namely with and without the inclusion of aromatic components. The adopted fuel surrogate models were developed from an integrated mechanism reduction scheme [2,3] and were well validated under wide range of shock tube and jet-stirred reactor conditions in zero-dimensional chemical kinetic simulations [4]. The core objective of this work will be separated into two parts. The first is to assess the validity of the numerical modelling approach through comparisons with experimental combustion characteristics and emissions of a light-duty diesel engine using single injection scheme. Parameters of the injection scheme will then be analysed, including the SOI timings. How these variations interact with the soot emission processes will be the key interest for this study.

2. Numerical formulations and setups
To ensure an effective mixing of fuel species with its surrounding gas phase, the renormalized group (RNG) k-ε model was used to model the in-cylinder turbulence. Subsequently, the Kelvin Helmholtz-Rayleigh Taylor (KH-RT) was implemented to model the droplet breakup process. To model the soot formation process, the Moss-Brookes model was used to determine the soot mass density.

As for the mesh configurations, the combustion chamber is modelled as a single cylinder, light-duty diesel engine, which includes a direct injection scheme that deliver fuel into the combustion chamber at specified injection timing. To illustrate, Table 1 outlines the engine specifications and conditions used to model the test engine. In terms of combustion model, a couple of multi-component diesel surrogate models will be used to simulate the internal engine combustion, namely through the surrogate models MCDS1 and MCDS2 [5]. The two models differ in terms of chemical kinetics that comes with different fuel constituents, specifically the inclusion of aromatic components in MCDS2. The details for fuel composition and properties of each model are provided in Table 2.

| Engine specifications | Operating conditions |
|-----------------------|----------------------|
| Bore × Stroke          | Engine speed         |
| 86 mm × 86 mm          | 1600 RPM             |
| Displacement           | Start of injection timing |
| 0.5 L                 | +2 ATDC              |
| Compression ratio      | Injection quantity   |
| 18.2 : 1              | 27.6 mg              |
| Nozzle orifice diameter| Initial temperature  |
| 0.149                 | 313 K                |
| Included spray angle   | Initial pressure     |
| 154°                  | 1.01 bar             |

Table 1. Engine specification and operation conditions.

| Properties                          | MCDS1                      | MCDS2                      |
|-------------------------------------|----------------------------|-----------------------------|
| Chemical formula (mass fraction)    | 0.42 HXN + 0.58 HMN        | 0.42 HXN + 0.20 HMN + 0.28 toluene + 0.10 CHX |
| Type of hydrocarbon                 | Straight- and branched-alkanes | Straight-, branched- and cyclo-alkanes, aromatic |
| Molecular weight                    | 226.446 g/mol              | 174.612 g/mol              |
| H/C Ratio                           | 2.125                      | 1.838                      |

Acronyms:- HXN: n-hexadecane, HMN: 2,2,4,4,6,8,8-heptaethylnonane, CHX: cyclohexane

The earliest injection timing was set to begin at 6° before the top dead centre, or SOI of −6 after top dead centre (ATDC) in short. The subsequent two injection profiles were set with four degree of delay interval, namely with the SOI timing positioned at −2° and +2° ATDC respectively. In general, changes in SOI timing will likely affect the combustion and soot formation process, as in-cylinder pressure and temperature vary measurably when reaching top dead centre in the compression stroke.

3. Validations of combustion model
Prior to studying the interactions between SOI timings and soot emission processes, the validity of the selected combustion model must be assessed beforehand, namely the combustion characteristics of surrogate fuel models in a three-dimensional (3-D) internal combustion engine. The analysis will be performed through comparisons with experimental data obtained from a light-duty diesel engine with similar operating conditions, where the simulated ignition delay (ID) timings and heat release rate (HRR) readings will be analysed. Figure 1 demonstrates the simulation results using various SOI timings. The simulated ID and HRR obtained from the combustion agree reasonably well with the experimental measurements. However, upon closer inspection, it can be observed that the ID of MCDS2 is slightly longer than of MCDS1, along with lower peak combustion pressure. Granted that one of the key differences between MCDS1 and MCDS2 is the inclusion of aromatic components, it is suggested that the lower cetane number of toluene in MCDS2 has made the fuel difficult to ignite.

Figure 1. Measured and simulated in-cylinder pressure/heat release readings for various injection timings, namely (a) SOI +2°, (b) SOI −2° and (c) SOI −6°.

4. In-cylinder soot formation events

It is of key interest to understand the interaction between SOI timing and in-cylinder soot formation, as shifting the injection profile could potentially reduce the soot yield through raising the combustion temperature. It is worth mentioning that fuel injection timing remains one of most accessible engine parameters to be calibrated. Figure 2 depicts the soot density yield associated with advancing the SOI timing from +2° to −6° ATDC. It can be seen that all three soot profiles have similar onset for soot formation corresponding to their SOI timing. Subsequently, both the peak and exhaust soot quantity have clearly decreased with advancing the SOI timing from +2° to −6° ATDC. This may be attributed
to the higher amount of fuel delivered with retarded SOI timing, in which more fuel consumption is required to maintain the constant power output [5]. Additionally, for the case of MCDS1, its net soot yield is consistently higher than of MCDS2. As discussed in the previous study [4], this can be attributed to the higher amount of straight- and branched- alkanes which promotes the production of the soot precursor species (i.e. C₂H₃). Next, the formation of soot particle involving multiple distinct stages, namely through soot nucleation, surface growth, and soot oxidation are analysed.

4.1. Soot nucleation

Inception of soot particle could be the main contributor of soot yield as they provide nucleation point for subsequent surface growth. In this study, C₆H₆ is designated as the soot precursor species for MCDS2 surrogate model, as CHX mechanism is integrated into the multi-component mechanism. On the other hand, C₂H₂ is selected for MCDS1 instead as it doesn’t contain Polycyclic aromatic hydrocarbons (PAH) chemistry. Figure 3 illustrates the nucleation profile for various SOI timings along with associated C₂H₂ mass fraction.

![Figure 2. Soot evolution profiles predicted for different injection timing, with the circles representing exhaust soot density measured at EVO respectively.](image)

![Figure 3. Effect of various SOI timings on the soot nucleation rate and the C₂H₂ mass fraction.](image)

From Figure 3, the highest nucleation rate is observed in the SOI −6 case, followed by SOI +2 and SOI −2. To begin with, it is likely that the higher soot inception for SOI −6 is caused by the enhanced reaction rate from increased temperature. In addition, it seems that the soot nucleation rate of MCDS1 is significantly higher than of MCDS2, probably due to the presence of additional C₂H₂ possessed by
MCDS1. It is possible that the higher amount of HMN used in the composition of MCDS1 could have increased the production rate of $\text{C}_2\text{H}_2$, which explains the higher soot yield gained from surface growth. Subsequently when compared to PAH, the higher mass concentration of $\text{C}_2\text{H}_2$ could have led to higher soot inception rate.

4.2. Surface growth

Surface growth can be described as the addition of gaseous hydrocarbons to the highly reactive surface of newly formed soot nuclei. When doing so, the soot particle often grows in size and experience mass gain from being adhered by other molecules. In general, the rate of surface growth is widely considered as the main contributor for total soot mass [9]. In any case, Figure 4 shows the surface growth profile for various SOI timing along with mean in-cylinder temperature. As shown in the result obtained in Figure 4, advancing the SOI timing from $+2^\circ$ to $-6^\circ$ ATDC has brought measurable effect to the soot surface growth rate. Additionally, for the case of SOI $-6$, its surface growth rate was found to be considerably higher than the other two. In other words, it is likely that advancing the SOI timing further away from the TDC has led to higher compression of cylinder charge. As a result, the fuel combustion took place in a relatively higher temperature which promote additional surface growth. Interestingly such event doesn’t occur for the case of SOI $+2$, as most of its fuel is delivered during the expansion stroke.

![Figure 4. Surface growth profile associated with various SOI timing, tagged along with mean in-cylinder temperature.](image)

4.3. Soot oxidation

Oxidation of soot involves reduction of soot mass by converting existing soot particle back into gaseous products such as CO and CO$_2$. In general, oxidation occurs near the soot surface and oxidize the carbon accumulated in the soot particles. Figure 5 below illustrates the oxidation profile associated with multiple SOI timings, together with associated OH mass fractions. It can be observed that production of OH radicals decreases with delayed SOI timing. Provided that OH is the main oxidizer under fuel-rich conditions [6], the lower amount of OH present could have led to lower soot oxidation rate. Furthermore, it was found that the formation of OH radicals continue to rise slightly despite the decrement in oxidation rate. As a result, the relatively long lifespan of OH radicals could have caused the small raise in oxidation rate observed during the mixing-controlled combustion (MCC) phase.
5. Conclusion

In this work, the combustion and soot formation characteristics of MCDS1 and MCDS2 surrogate model are studied, particularly under the conditions of a light-duty, direct-injection diesel engine setup. It is demonstrated that advanced injection timing (i.e. -6° after top dead centre) has contributed to reduced soot emission as compared to retarded injection timing. While both the soot inception, surface growth and oxidation rate show sign of increase with earlier start of injection timings, it is likely that the oxidation rate increases faster under high temperature conditions, thus leading to lower overall soot yield. When compared to MCDS2 model, it was observed that the combustion of MCDS1 has consistently led to higher soot yield across all the cases. While the inclusion of aromatic components should have promoted soot formation, it is possible that the higher amount of C_2H_2 in MCDS1 could have accelerated the inception of soot particles. The study here provides a better understanding of the effects of fuel injection timings that govern the soot production and oxidation processes in a light-duty, direct-injection diesel engine.

References

[1] Mohan B, Yang W and Chou S K 2013 Fuel injection strategies for performance improvement and emissions reduction in compression ignition engines—A review Renew Sustain Energy Rev 28 664.

[2] Poon H M, Ng H K, Gan S, Pang K M and Schramm J 2014 Development and validation of chemical kinetic mechanism reduction scheme for large-scale mechanisms SAE Int J Fuels Lubr 7 653.

[3] Poon H M 2016 Development of integrated chemical kinetic mechanism reduction scheme for diesel and biodiesel fuel surrogates for multi-dimensional CFD applications Thesis University of Nottingham.

[4] Poon H M, Pang K M, Ng H K, Gan S and Schramm J 2016 Development of multi-component diesel surrogate fuel models - Part II: Validation of the integrated mechanisms in 0-D kinetic and 2-D CFD spray combustion simulations Fuel 181 120.

[5] Pang K M, Ng H K and Gan S 2012 Investigation of fuel injection pattern on soot formation and oxidation processes in a light-duty diesel engine using integrated CFD-reduced chemistry Fuel 96 404.

[6] Bowman C T, Bartok W and Sarofim A F 1991 Fossil Fuel Combustion-A source Book.