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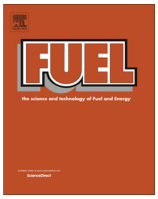

Application of a semi-detailed soot modeling approach for conventional and low temperature diesel combustion – Part I: Model performance

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HIGHLIGHTS

- CFD-based soot model was tested for conventional diesel combustion, LTC, and PCCI.
- Model can be used for soot mass, number density, and particle diameter predictions.
- Soot particle size is larger for high temperature combustion conditions.
- Soot particle size is lower for LTC through-out the combustion process and at EVO.

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ABSTRACT

In the present study a previously developed soot model has been tested extensively for conventional and low temperature diesel combustion engine simulations. The soot model framework, which was implemented in the Computational Fluid Dynamics (CFD) code KIVA-CHEMKIN, is based on four fundamental steps, viz., soot inception through a four ring polycyclic aromatic hydrocarbon species, soot surface growth through acetylene and benzene, soot coagulation, and oxygen and OH-induced soot oxidation. The proposed model can be used not only for soot mass predictions, but also for soot number density and soot particle diameter predictions. Diesel combustion was simulated using reduced n-heptane/primary reference fuel (PRF) chemistry mechanisms and a reduced polycyclic aromatic hydrocarbon (PAH) chemistry mechanism, while the n-heptane chemistry mechanism was used for modeling constant volume n-heptane combustion. Soot model performance was evaluated by comparing the model predictions with available constant volume combustion chamber optical diagnostic experiments, optical engine in-cylinder soot data, and a light-duty single cylinder metal engine-out smoke data. In particular, a variety of combustion regimes were tested, including conventional diesel, premixed charge compression ignition (PCCI), and high exhaust gas recirculation (EGR) low temperature combustion (LTC). In general, the model was able to predict well the trends in soot mass over the range of operating conditions. With increasing degree of premixing, the model was able to predict relatively lower soot concentrations compared to diffusion combustion. In terms of soot particle diameter, the model computed particle size was seen to increase with increasing simulated EGR when the ambient oxygen concentration was varied from 21% to 8% by volume and with increasing in-cylinder density (14.8 kg/m^3 vs. 30 kg/m^3 at the same in-cylinder O_2 level) under steady-state constant volume combustion conditions. It is also observed from the optical and metal engine studies that the soot particle size is larger for high temperature combustion conditions that are marked with high soot formation rates during the combustion process and may or may not lead to smaller particles at exhaust valve opening (EVO) depending on the oxidation rates. The soot size for LTC is generally lower through-out the combustion process including EVO conditions. All but one data-point show uni-modal type soot particle size distribution with respect to both soot mass and particle number.

1. Introduction

Increasingly stringent pollution mandates have necessitated further study of gasoline and diesel combustion fundamentals. Particularly, mitigating emissions of NOx and soot in diesel engines

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has been a long-standing challenge for the internal combustion engine community. After-treatment devices such as selective catalytic reduction (SCRs), NOx absorbers and diesel particulate filters (DPFs) are actively being employed to control regulated pollutant emissions, but the conversion efficiency, durability, backpressure, and the need for thermal management strategies are some of the challenges posed by these devices. Also, with recent emphasis on corporate average fuel economy (CAFE) and greenhouse gas (GHG) standards, the spotlight in engine research has lately transitioned from emissions to fuel economy. Hence there exists a need to probe alternative combustion strategies, not only to reduce emissions within the engine combustion chamber, but also from an efficiency standpoint. These advanced combustion strategies are significantly different than conventional combustion strategies for both spark-ignited (SI) and compression-ignited (CI) engines. Particularly for diesel engines, strategies such as homogeneous charge compression ignition (HCCI), achieved by significantly early injections, premixed charge compression ignition (PCCI), possibly with two injections (one early and one conventional), and low temperature combustion (LTC) with heavy amounts of exhaust gas recirculation (EGR) are being explored [1,2]. Fig. 1, reproduced from Akihama et al. [1] and modified here (shown in bold text) for illustration purposes, shows the combustion regimes in the classic equivalence ratio-temperature (Φ–T) map. The modifications were based on the generic Φ–T plot shown in Tree and Svensson [2], which are derived from the experimental observations of Pickett and Siebers [3] in a constant volume spray vessel. These regimes of combustion are very different compared to conventional diesel diffusion combustion, which significantly alters the mechanisms of pollutant formation processes. As seen in Fig. 1, the drive has been to operate the engine either between the soot and NOx peninsulas or at much lower temperatures, which provides a wider operating range and hence is desirable. Soot formation can be avoided either by operating at lower temperatures (<1800 K) or higher temperatures (>2600 K) or lower local equivalence ratios (<2), but lower NOx warrants lower in-cylinder temperatures. Points 1 (a) and 1 (b) refer to high EGR LTC (~10% ambient O_2) with a small nozzle diameter (~50 μ) for enhanced fuel–air mixing. The fuel jet core is represented by point 1a ($\Phi > 1$ and low temperature) while the flame sheet is represented by 1b ($\Phi \sim 1$ and high temperature). As the nozzle diameter is small, which enhances atomization, the entrained air amount is higher, which inhibits soot formation in the fuel jet core. In the flame sheath region the high EGR helps to keep the temperatures low and hence lower in-cylinder NOx is achieved. Point 2 corresponds to an ambient temperature of 850 K with higher oxygen content (21% O_2) and also using small nozzle diameters (~50 μ). This corresponds to low temperature lean combustion. PCCI falls closer to point 2, which is generally accomplished with multiple injections where the overall equivalence ratio could be much less than local equivalence ratios. The ordinate of the point 'PCCI' in the figure represents the local equivalence ratio. Point 3 refers to high EGR operation (~8% ambient O_2) with a production feasible nozzle diameter (~180 μ) while operating with an oxygenated fuel, which produces the same result of low NOx and low soot.

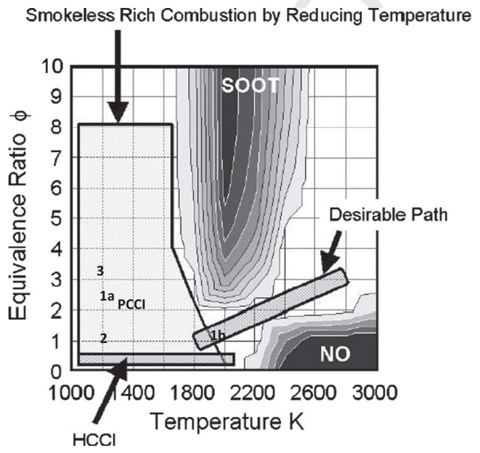

Fig. 1. Generalized Φ–T map showing HCCI, PCCI and LTC regimes of operation (original figure from Akihama et al. [1] and modified based on Tree and Svensson [2]).

This discussion indicates that there are multiple ways of obtaining low NOx and low soot, at least from a scientific standpoint, and the current techniques rely on longer ignition delay combustion strategies to allow more time for fuel–air mixing. From a modeling perspective, predicting emissions for low NOx-low soot combustion necessitates less empirical and more physically driven pollutant models that can reasonably replicate the formation and oxidation kinetics over a wide range of operation. Particularly, soot modeling for conventional diesel combustion has been a long standing research subject and, with newer combustion regimes, soot models are further challenged. Also, to prevent the possibility of allowing ultra-fine particles from escaping into the atmosphere, future US, Japan and European standards aim at mandating particulate number (PN) (Johnson [4]), and thus model predictions of engine-out soot particle size and number density along with soot mass have gained increasing importance.

Finally, the last piece of the modeling puzzle is the fuel itself. Due to limited resources of fossil fuels and with the growing momentum for their conservation, dual fuel combustion such as pilot diesel ignited natural gas, reactivity controlled compression ignition (RCCI) [5], and use of alternative fuels such as E85 (85% by volume of ethanol and 15% by volume of gasoline) and biodiesel are also being explored for diesel and gasoline engines. The pathways of soot formation differ from one fuel to another depending upon the fuel composition. Regular pump gasoline or diesel may have anywhere between 20% and 32% aromatics by volume, which are also major contributors to soot formation, in addition to soot formation due to fuel chain breakdown. However, fuels such as biodiesel (mainly composed of fatty acid esters) and natural gas (mainly composed of methane) do not have fuel aromatics and hence the soot formation is directly a function of the fuel breakdown chemistry. Thus, newer emission and fuel efficiency standards along with the continued focus on exhaust particulate reduction motivate the drive toward newer in-cylinder engine combustion strategies and alternative fuels. Consequently, the modeling thrust is to reduce empirical approaches and replace them with more physics-based detailed and versatile combustion and emission models.

In the present work, the soot model of Ref. [8] implemented in the 3-D CFD code KIVA-CHEMKIN was applied to study advanced diesel combustion modes, including conventional diesel combustion, high-EGR diesel LTC and diesel PCCI. Also, the model predictions of soot mass were compared with available experimental data and model predictions of soot diameter were qualitatively evaluated for each combustion mode. The computational mesh, spray, turbulence, and other sub-models are the same as used in Vishwanathan and Reitz [8].

2. Model framework

2.1. Chemistry mechanisms

2.1.1. Fuel and lower carbon chemistry

Two separate chemistry mechanisms were used in the present study. The first mechanism (Mech-1) comprised 37 species and

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