

Simulation and Analysis of In-Cylinder Soot Formation in a Low Temperature Combustion Diesel Engine Using a Detailed Reaction Mechanism

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ABSTRACT

3-D Computational Fluid Dynamics (CFD) simulations have been performed using a detailed reaction mechanism to capture the combustion and emissions behavior of an IFP Energies Nouvelles optical diesel engine. Simulation results for in-cylinder soot volume fraction (SVF) have been compared to experimental data reported by Pires da Cruz et al. [1] for the engine operating in low-temperature combustion (LTC) mode with high EGR, and for varied operating conditions. For the simulations, a 4-component surrogate blend containing n-hexadecane, heptamethylnonane, 1-methylnaphthalene, and decalin was used to represent the chemical and physical properties of the standard European diesel used in the engine tests. A validated detailed surrogate mechanism containing 392 species and 2579 reactions was employed to model the chemistry of fuel combustion and emissions. In addition, a new pseudo-gas soot model was developed and coupled with the fuel chemistry to simulate in-cylinder soot nucleation, growth, and oxidation processes. A 60° sector mesh containing 53500 cells was used for the engine simulations using the FORTÉ CFD simulation software. Comparisons of calculated in-cylinder soot volume fractions to those measured show good agreement for crank-angle-resolved SVF. Soot production nominally begins as soon as the combustion starts around 6 crank angle degrees (CAD) after TDC, and peaks approximately 12 CAD after TDC when soot oxidation begins to dominate. Simulations captured the location of soot in the center of the bowl just above the wall, and trends in SVF with variation in operating parameters, including fuel loading, EGR, injection timing, and intake temperature. Advancing injection timing and increasing fuel loading increases peak soot levels, whereas lower EGR and lower intake temperatures lower peak soot levels. Simulations also capture the trends in other emissions for varied operating conditions. Further analyses have been performed to understand the combustion and emissions processes.

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INTRODUCTION

Emissions regulations are expected to continue being more stringent in coming years. Various strategies are being considered for emissions control, including low-temperature combustion (LTC) modes for diesel engines. The LTC mode typically is achieved via late fuel injection and a high level of exhaust gas recirculation (EGR). Peak temperatures in LTC diesel engines are lower than those in conventional engines, which help lower NO_x emissions. However, lower operating temperatures may adversely impact emissions by increased soot emissions at lower temperatures. Pires Da Cruz et al. [1] at IFP Energies Nouvelles (IFPEN) constructed a single-cylinder optical engine to study soot formation in LTC mode. They measured the location of soot formation and its volume

fractions inside the cylinder at various crank angles using laser induced incandescence and extinction techniques. They also varied several engine operating conditions one at a time to observe their impact on soot emissions.

The goal of this work is to simulate those engine experiments to capture the in-cylinder soot formation and destruction as observed by Cruz et al., and to accurately capture the impact of engine operating conditions on soot using 3-D computational fluid dynamics (CFD). Since fuel reactivity is typically lower at the low temperatures of the LTC engine mode, kinetics play a more important role for the LTC mode than for a conventional diesel engine. Therefore, accurate fuel reaction mechanisms are needed to model the LTC diesel engine and to understand the combustion and emissions processes. Only recently it has become possible to



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use detailed reaction mechanisms in 3-D engine CFD simulations [2]. In this study, a detailed reaction mechanism with a multi-component surrogate diesel fuel has been employed in the CFD simulation to accurately model fuel combustion and emissions chemistry including soot.

Most soot models widely used in CFD today are one- or two-step models. These are semi-empirical soot models [3] that have been calibrated based on limited data. Though some recent studies attempted to improve such soot models [4] they are limited by the accuracy or applicability of the gas-phase combustion mechanism coupled with the soot model. In conjunction with using a detailed and well validated gas-phase fuel combustion mechanism in this work, we have proposed a new pseudo-gas-phase soot model. This is a simplified soot model that describes all the important soot formation and oxidation mechanisms. The following sections describe the engine in brief, followed by the model descriptions, simulation setup, results, and analyses.

ENGINE AND SIMULATION SETUP

We used the FORTÉ CFD Simulation Package [5], which allows the use of large reaction mechanisms, to achieve an accurate description of fuel combustion and soot-precursor formation. Specifications of the optical engine are described in detail elsewhere [1] and summarized in Table 1. A 6-hole common rail fuel injector was used in the experiments. A 60-degree sector mesh was generated and used to represent the cylinder geometry with 53500 cells at BDC.

Engine Operating Conditions and Parametric Variations

The IFPEN diesel engine is operated under LTC mode. The engine was operated at 1200 RPM under fuel-lean conditions with fuel-air ratio of 0.34 and high EGR. The reference or baseline conditions were inlet temperature of 69 °C, SOI 353 CAD, injection duration of 3.5 CAD, 35% simulated EGR via nitrogen dilution, and IMEP of 2.5 bar (i.e., low-load conditions).

Table 1. IFPEN optical engine characteristics.

Optical Single-cylinder Engine	
Number of cylinders	1
Cycle	4 stroke
Number of intake valves	2
Number of exhaust valves	1
Combustion	Flat optical bowl
Cylinder head type	Flat
Displacement	499.3 cm ³
Bore	85 cm ³
Stroke	88 mm
Connecting rod length	144 mm
Compression ratio (measured)	12.8:1
Swirl at BDC	2.2
Injection system	Common Rail Bosch

Four additional experiments were performed by changing one parameter at a time from the reference conditions. These variations included (1) advanced SOI of 351 CAD, (2) higher IMEP of 3 bar, (3) lower EGR of 30%, and (4) lower intake temperature by 7 °C - as listed in Table 2. For the modeling, the mesh-independent physical model constants, including those for the spray, break-up, and vaporization, as well as the turbulence models, were all kept at their software-default values. This provides a good test for the model's capability to capture the parametric variations in engine.

Table 2. Parametric variations for the engine operating conditions.

Parameter	Change from reference conditions
Reference	-
SOI	351 CAD (reference 353 CAD)
IMEP	3 bar (reference 2.5 bar); 20% more fuel injected than reference
EGR	30% (reference 35%)
T _{inlet}	62 °C (reference 69 °C)

Fuel Surrogate and Reaction Mechanism Used in CFD

A multi-component surrogate blend was generated for representing the fuel chemistry of the European diesel with Cetane Number of 54 that was used in the engine experiments. Available fuel properties are shown in Table 3. The components in the surrogate were chosen with the aim to represent the chemical composition and combustion properties of diesel, and to a lesser extent its physical properties. The Surrogate Blend Optimizer software [6], which is a part of Reaction Workbench [7], was used to optimize the composition of the blend. Components' detailed reaction mechanisms were obtained from the Model Fuels library [8] database that contains validated mechanisms for over 40 liquid and gaseous fuel components that can be used to formulate surrogates for gasoline, jet fuel, diesel, and biofuels. All the fuel component mechanisms from this library have self-consistent and extensively validated reaction mechanisms [9]. The optimized surrogate contains 4 components as shown in Table 4. Estimated properties of the surrogate as shown in Table 3 match those of European diesel well.

Table 3. Surrogate Blend Optimizer targets and resulting properties of the surrogate.

Property	Target	Surrogate
Cetane Number	54	54
Molar H/C Ratio	1.875	1.87
Liquid Density, g/cm ³	0.834	0.8271
L.H.V., MJ/kg	-	43.76
T ₅₀ , K	-	498.5

The master detailed mechanism from the Model Fuels library for diesel surrogates contains more than 4000 species and over 16000 elementary reactions. The master mechanism has been extensively validated to confirm accurately predictions of autoignition times, as well as emissions including CO, NO_x, UHC, and PAH [9,10,11,12,13].

Table 4. Proposed surrogate for the standard diesel used in IFPEN engine tests.

Component	Mass %
<i>n</i> -Hexadecane	36.03
1-Methylnaphthalene (AMN)	9.71
Heptamethylnonane	15.37
Decalin	38.89

For this work, a new pseudo-gas phase soot model has been developed to be used with the detailed mechanism to predict soot fractions. The mechanism has been developed based on our findings from development of a more detailed soot reaction mechanism. As highlighted in Figure 1, the overall scheme for soot generation is a result of fuel combustion that forms fragmented hydrocarbons under fuel-rich conditions that generate PAH. Soot nucleates from large PAHs and then grows by addition of acetylene and other smaller PAH molecules. In order to simplify the soot mechanism for CFD applications, we have created a multi-step pseudo-gas soot model that works with a detailed mechanism for fuels. Steps in the soot model are shown in Table 5. The nucleation is assumed to be formed from the 1st aromatic ring species. This is a reasonable approximation since formation of the 1st ring is the rate-limiting step in PAH formation that eventually leads to soot. Unlike other studies that use pyrene for nucleation, this approach does not require a very large gas phase mechanism. Typical uncertainty in the gas phase mechanism is higher for the PAH growth chemistry, and using the 1st aromatic ring species for soot nucleation avoids the need for accurate PAH growth chemistry in the gas phase. Primary particles are described by the species NUCL in the model. Further growth is achieved from multi-step soot growth reactions involving acetylene and benzene. Finally, several soot oxidation steps are included in the model. In addition, oxidation from NO₂ and sensitization from H₂O steps are included. The soot model is initially calibrated using the measurements from a burner-stabilized-stagnation-flow (BSSF) flame for ethylene from Wang and co-workers [14,15,16]. Then it is further tuned to match the peak soot level from the engine measurements at the reference operating condition. No other adjustments are made and the same rate parameters are used for all simulations.

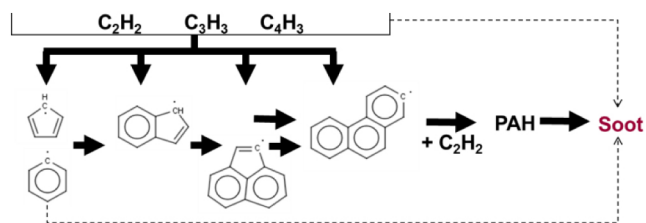


Figure 1. Sketch for PAH growth from hydrocarbons that lead to soot formation based on detailed reaction mechanism for fuel combustion and PAH generation.

Table 5. Steps in the new pseudo-gas soot model. C.f. text for the description.

Reaction	Importance
$C_6H_6 + C_6H_5 = 0.375 \text{ NUCL} + 5.5 \text{ H}_2$	Nucleation
$C_2H_2 + \text{NUCL} = \text{NUCL} + 0.0625 \text{ SOOT} + \text{H}_2$	Growth
$C_6H_6 + \text{NUCL} = \text{NUCL} + 0.1875 \text{ SOOT} + 3 \text{ H}_2$	Growth
$0.03125 \text{ SOOT} + \text{OH} = \text{CO} + 0.5 \text{ H}_2$	Oxidation
$0.0625 \text{ SOOT} + \text{O}_2 = 2 \text{ CO}$	Oxidation
$0.03125 \text{ SOOT} + \text{NO}_2 = \text{CO} + \text{NO}$	Oxidation
$\text{H}_2\text{O} + \text{SOOT} = \text{OH} + 0.5 \text{ H}_2 + \text{SOOT}$	Sensitization

Although large mechanisms with thousands of species can be used in FORTÉ CFD simulations, the compute time will still be very long for practical applications. Therefore, we reduced the master mechanism using Reaction Workbench software [7]. Several mechanism reduction methods have been implemented in the software and their capabilities have been highlighted in our previous publications [6]. In brief, Reaction Workbench uses any ideal reactor model in CHEMKIN-PRO [17]. It automatically generates a smallest mechanism for a given tolerance on targets such as autoignition times, flame speeds, species concentrations, etc., that are calculated by CHEMKIN-PRO under appropriate reactor conditions. In this work, we used a closed homogeneous reactor for the mechanism reduction for the surrogate composition, and with accuracy targets to maintain 10% accuracy on autoignition times and concentration of several important species. A parametric study covering a broad range of temperatures, pressures, equivalence ratios, and dilution was set up for the mechanism reduction project in CHEMKIN-PRO and used by Reaction Workbench for the mechanism reduction.

Reduction methods including DRG, DRG-EP, isomer lumping, and sensitivity analysis were used in iterative fashion to reduce the master mechanism to the smallest size while maintaining the accuracy within the acceptable tolerance over a broad range of conditions. The resulting reduced yet detailed reaction mechanism for the surrogate diesel contains 392 species. Simulation from IVC to EVO with this mechanism in CFD with the 53500-cell sector mesh took approximately 21 hours on an 8-core Intel Xenon machine.

VALIDATION OF THE REACTION MECHANISM

Prior to using the 392 species mechanism for the 4-component European diesel surrogate in CFD simulations, we performed validation using the fundamental experimental data available for diesel and for major components in the surrogate. Various published data using jet-stirred reactor, shock-tubes, and BSSF flames are used for validation. All simulations were performed using ideal reactor models in CHEMKIN-PRO [17]. Results for selected and most relevant data sets are presented in this section.

Ramirez et al. [18] measured profiles of various products in a jet-stirred reactor during oxidation of a European diesel at 10 atm and for equivalence ratio of 1.5. Reactor temperature was varied from 550 K to 1050 K. The residence time in the reactor was 1 s. Since the diesel used was similar to the one used in engine experiments with Cetane Number with 1 number, we used the same surrogate blend shown in Table 4 for simulation of these experiments. Comparison of predicted profiles of CO and formaldehyde to those measured are shown in Figure 2 and Figure 3 respectively. Predictions using the master mechanism with over 4000 species, and those using the 392 species mechanism for diesel are in good agreement with the data and with each other. The mechanisms also accurately capture the negative temperature coefficient region between 650 K and 750 K where reactivity decreases with increase in temperature.

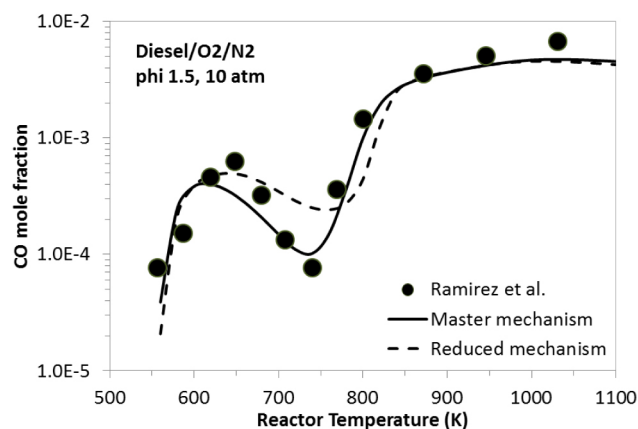


Figure 2. Predicted CO profiles compared with the jet-stirred reactor data of Ramirez et al. [18] for a diesel/O₂/N₂ mixture. Lines are simulation results and symbols are experimental data. Conditions include a pressure of 10 atm, residence time of 1 s and phi of 1.5 (~99 mol% N₂ dilution).

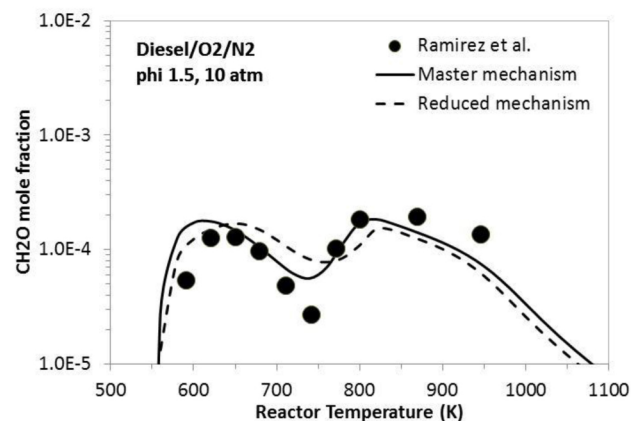


Figure 3. Predicted formaldehyde (CH₂O) profiles compared with the jet-stirred reactor data of Ramirez et al. [18] for a diesel/O₂/N₂ mixture. Lines are simulation results and symbols are experimental data. Conditions include a pressure of 10 atm, residence time of 1 s and phi of 1.5 (~99 mol% N₂ dilution).

Haylett et al. [19] measured time resolved profiles of ethylene and OH produced during oxidation of n-hexadecane in an aerosol shock-tube. Experimental conditions were 1333 K, 6.8 at, equivalence ratio of 1.2. Comparison of predicted species profiles to those measured is shown in Figure 4. Predictions agree well with the measurements. Predictions using the master and reduced mechanisms are virtually indistinguishable for the most reactive component in the surrogate which is also in the highest amount in the blend (Table 4).

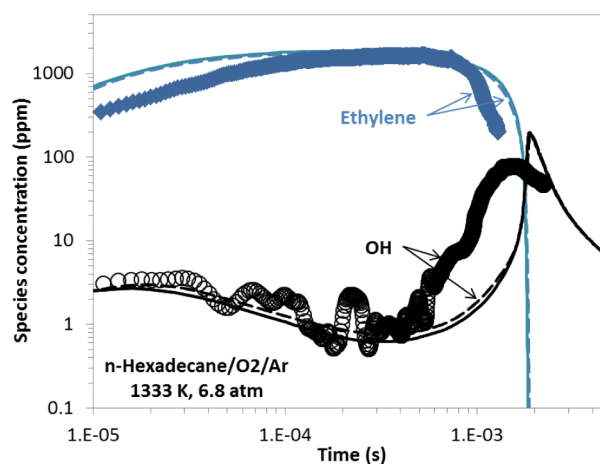


Figure 4. Calculated species profiles of ethylene and OH, compared with the shock-tube reactor experimental data of Haylett et al. [19] for 493 ppm n-hexadecane /10000 ppm O₂/Ar (phi 1.2). Symbols are experimental data, solid lines represent predictions using the master mechanism, and dashed lines represent predictions using the reduced mechanism.