

Effects of EGR on soot processes in n-dodecane spray combustion at high ambient temperature

Min Zhang^{1*}, Jiun Cai Ong¹, Kar Mun Pang², Xue-Song Bai³, Jens Honore Walther^{1,4}

1 Department of Mechanical Engineering, Technical University of Denmark, 2800 Kgs. Lyngby, Denmark

2 Man Energy Solution, Teglholmegade 41, 2450 Copenhagen, Denmark

3 Division of Fluid Mechanics, Lund University, P.O. Box 118, S221 00 Lund, Sweden

4 Computational Science and Engineering Laboratory, ETH Zürich, CH-8092 Zürich, Switzerland

ABSTRACT

This paper presents the numerical results of soot evolution in a constant volume chamber under different exhaust gas recirculation (EGR) levels at an ambient temperature of 1100 K by employing a two-equation soot model. The contribution and significance of each soot process on the net soot mass production are investigated. The numerical setup is able to capture the experimentally observed monotonic trend of the soot mass, in which soot mass increases with decreasing oxygen (O_2) level. The simulation results demonstrate that soot oxidation rates, particularly by hydroxyl radicals (OH), are the more dominating factors to the monotonic trend as compared to the inception and surface growth rates under different EGR.

Keywords: EGR, high ambient temperature, soot formation, soot oxidation

NONMENCLATURE

Abbreviations

EGR	Exhaust Gas Recirculation
ECN	Engine Combustion Network
LPL	Liquid Penetration Length
VPL	Vapor Penetration Length
IDT	Ignition Delay Time
LOL	Lift-off Length
CCM	Chemistry Coordinate Mapping
ASOI	After Start of Injection

Symbols

T_{am}	Ambient Temperature
$C_{12}H_{26}$	<i>n</i> -dodecane
OH	Hydroxyl Radical
O_2	Oxygen
C_2H_2	Acetylene

1. INTRODUCTION

Diesel engines are the main power source for large ships and heavy-duty vehicles. However, high soot emissions from diesel engines cause serious health and environmental problems. This results in a more stringent emission standard. Therefore, reduction of soot emission from diesel engines are crucial. Exhaust gas recirculation (EGR) in diesel engines is one of the approaches to reduce the soot emissions [1-3]. The soot mass at quasi steady-state varies in a non-monotonic manner as the EGR level increases. This can be explained by the slow soot formation process at low flame temperature resulted from high EGR level [1]. However, the variation of soot mass with EGR levels changes as the ambient temperature (T_{am}) increases [4].

Skeen et al. [4] investigated experimentally the soot processes over a range of T_{am} (800 K-1200 K) using *n*-dodecane ($C_{12}H_{26}$) as fuel and found that the variation of total soot mass with EGR differs at different T_{am} . When the T_{am} is higher than 1050 K, the total soot mass shows a monotonic trend such that the total soot mass increases with increasing EGR level. A numerical study performed by Wang et al. [5] was able to capture this

monotonic trend at 1100 K. Despite capturing the monotonic trend, no detail explanation was presented in the literature. As such, the present study aims to gain a better understanding of the effects of EGR on soot formation and oxidation at the T_{am} of 1100 K. A phenomenological soot model which accounts for the soot inception, coagulation, surface growth as well as oxidation by both hydroxyl radical (OH) and oxygen (O_2) [6], is used.

2. NUMEERICAL FORMULATION AND SETUP

Engine Combustion Network (ECN) Spray A is simulated in this study where $C_{12}H_{26}$ is injected at a pressure of 150 MPa through a nozzle in diameter 90 μm [7]. T_{am} and the ambient density are fixed at 1100 K and 22.8 kg/m³, respectively. The O_2 levels are set to 13%, 15% and 21% to represent different EGR levels. The simulation work is performed using OpenFOAM-v1712. The computational domain is a cube with a length of 108 mm for each side. A uniform mesh size of 0.25 mm is implemented in a refined mesh region (24 mm radially and 108 mm axially from the nozzle location) with a lower resolution closer to the walls. The computational time step is 0.2 μs . Second-order schemes are used for the spatial and time discretizations. Primary breakup is considered by sampling computational parcels from the Rosin-Rammler size distribution [8]. The Reitz-Diwakar model, with the stripping breakup constant calibrated to 8, is implemented to model the secondary break-up of the droplets [9]. The turbulence flow in the domain is simulated using the realizable k- ϵ model [10], where the constant C_2 is tuned to 1.8. The well-stirred reactor combustion model coupled with Chemistry Coordinate Mapping (CCM) [11] is used to account for the turbulence-chemistry interactions. Details about CCM are available in [11]. The reduced mechanism developed by Yao et al. [12] with 54 species is chosen. The two equation, phenomenological soot model developed by Pang et al. [6] is employed. The source terms of these two equations are able to account for soot processes including soot inception, coagulation, surface growth as well as soot oxidation due to OH and O_2 . These soot processes are modeled by global reactions, where the formula and constants are available in [6]. In this model, acetylene (C_2H_2) is selected as the soot precursor for inception and gas phase molecule of adsorption for surface growth.

3. NUMEERICAL FORMULATION AND SETUP

3.1 Validation of non-reacting and reacting spray

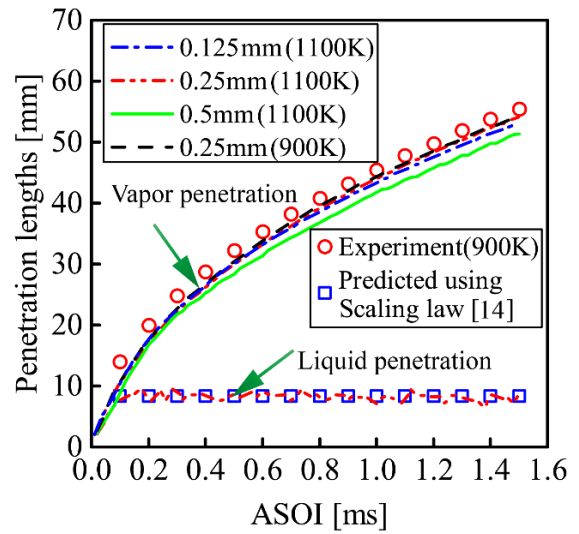


Fig 1 Liquid and vapour penetration lengths after the start of injection (ASOI).

The liquid penetration length (LPL) and vapor penetration length (VPL) for different mesh size and temperatures are shown in Fig. 1. Three different mesh sizes (0.5 mm, 0.25 mm and 0.125 mm) are used to study the grid independence. As depicted in Fig. 1, mesh size of 0.25 mm and 0.125 mm have reached grid independent. Considering a balance between accuracy and computational time, the mesh size of 0.25 mm is used in all subsequent simulations. Figure. 1 also shows that increasing T_{am} has no effect on VPL, which agrees with the experimental findings [13]. Due to the lack of measured LPL at 1100 K, the predicted LPL is compared against the LPL obtained from the scaling law method [14], which shows comparable results between them.

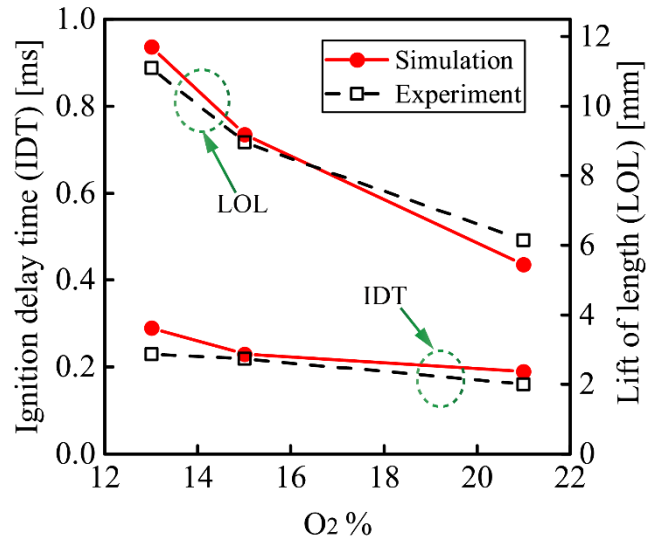


Fig 2 Comparison of ignition delay time (IDT) and lift-off length (LOL) between measured and simulation results.

In the present study the ignition delay time (IDT) is defined as the time when the rise rate of maximum

temperature reaches the maximum value [15]. The lift off length (LOL) is defined as the shortest distance from the injector where the OH concentration reaches 2% of its maximum value [15]. The computational and measured IDT and LOL at 1100 K for different O_2 levels are shown in Fig. 2. The computed IDT and LOL show a reasonably good agreement with the experimental data. The maximum relative error is 26.1% and 12.4% for IDT and LOL, respectively.

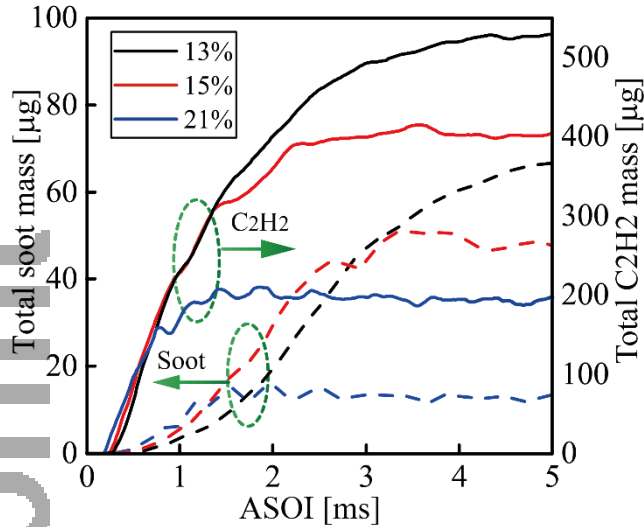


Fig 3 The evolution of total soot mass and total C_2H_2 mass.

3.2 Effect of EGR on soot evolution

The soot formation process is analyzed by comparing the predicted soot-relevant quantities at different EGR levels. Figure 3 depicts the evolution of total soot mass and total C_2H_2 mass within the whole domain using different O_2 levels of 13%, 15% and 21%. As shown in Fig. 3, the total soot mass shows a monotonic trend where the total soot mass increases with increasing EGR levels. The ratio among simulated total soot mass of 13%, 15% and 21% O_2 at quasi steady-state is 4.9:3.5:1 [4], while the measurement ratio is 2.9:2.5:1. Fig. 3 also shows that the higher O_2 level leads to a shorter time for total soot mass to reach quasi steady-state. This could be explained by the fact that the flame stabilizes at its lift-off distance more quickly at higher O_2 level. The total C_2H_2 mass shows a similar trend as the total soot mass. The ratio of the total soot mass to the total C_2H_2 mass at 5 ms is calculated as 12.6%, 11.8% and 6.9% for O_2 levels of 13%, 15% and 21%, respectively. It should be noted that this ratio is almost similar for 13% and 15% O_2 , but is much lower for 21% O_2 . This indicates that the total soot mass does not solely depend on the amount of C_2H_2 formed. The total OH mass for 21% O_2 is significantly higher than those

at lower O_2 levels (not shown in the paper). Therefore, higher OH oxidation rate and lower concentration of C_2H_2 are likely the reasons for the relatively lower total soot mass for 21% O_2 . This will be further verified in the next paragraph. As aforementioned, the total soot mass of 13% O_2 is higher than that of 15% O_2 . The soot inception and coagulation processes determine the soot number density and further influence the effective surface area, which in turn indirectly affects the total soot mass. An analysis of the total soot particle number as depicted in Fig. 4 shows that the total soot particle number for 13% O_2 and 15% O_2 are comparable to each other, in which both are higher than that in 21% O_2 . Therefore, when T_{am} is 1100 K and O_2 level is less than or equal to 15% O_2 the number of soot particle contributed by inception and reduced through coagulation may not be the main reason for the difference in total soot mass. This finding contradicts the results at 1000 K from [3] where the difference in total soot mass is mainly due to the huge difference in the number of soot particle when the O_2 level is less than or equal to 15% O_2 .

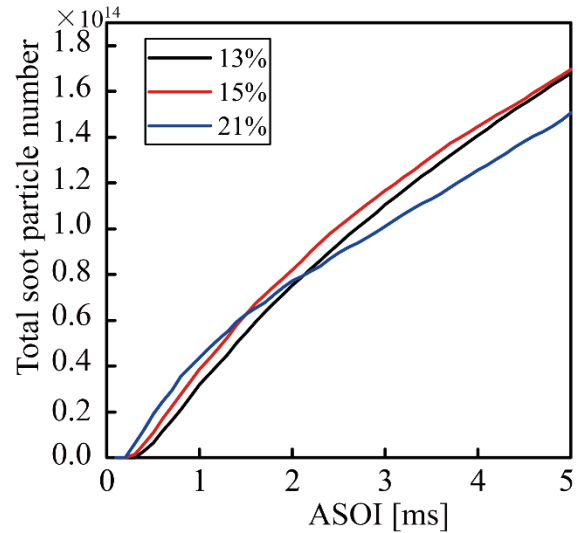


Fig 4 The evolution of total particle number under different EGR levels.

The effects of EGR on the individual soot processes are also investigated. Figure 5 shows the evolution of soot mass contributed from inception and surface growth under different EGR levels. Furthermore, Figure 6 shows the evolution of soot mass oxidized by OH and O_2 under different EGR levels. The soot mass contributed by surface growth for 21% O_2 is lower than other two cases, while the soot mass oxidized by OH for 21% O_2 is higher than other two cases. This further explains the lower soot mass for 21% O_2 in Fig. 3. One can see that the soot mass gained through surface growth for 15%

O_2 is higher than 13% O_2 (cf. Fig. 5), whereas the total soot mass of 15% O_2 is lower than that of 13% O_2 (cf. Fig.3). This is attributed by the fact that the soot mass oxidized by OH for 15% O_2 is significantly higher than 13% O_2 as shown in Fig. 6. In terms of oxidation by O_2 ,

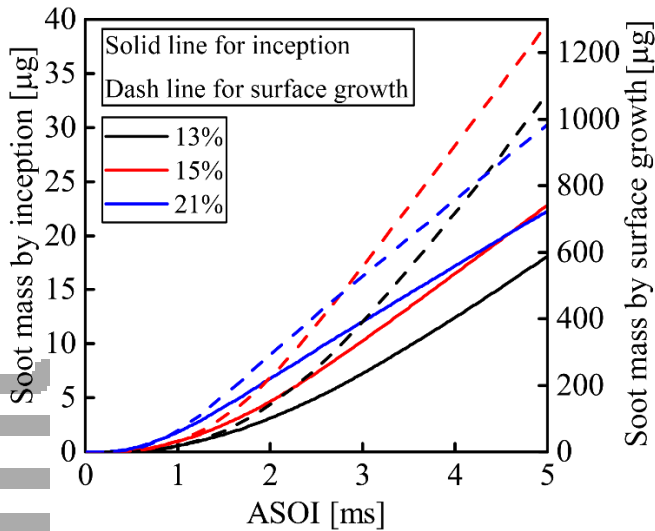


Fig 5 The evolution of soot mass contributed by inception and surface growth under different EGR levels.

the soot mass oxidized by O_2 for different EGR levels is comparable during the early 2 ms ASOI (after the start of injection). However, the soot mass oxidized by O_2 is significantly lower for 21% O_2 after 2 ms of ASOI. Based on the current formulation [6], oxidation by O_2 highly depends on the effective surface area of collision between soot and O_2 . The distribution of O_2 exists on the periphery of soot (not shown in the paper). As such, the associated effective surface area of collision between soot and O_2 is lower for 21% O_2 due to its smaller soot

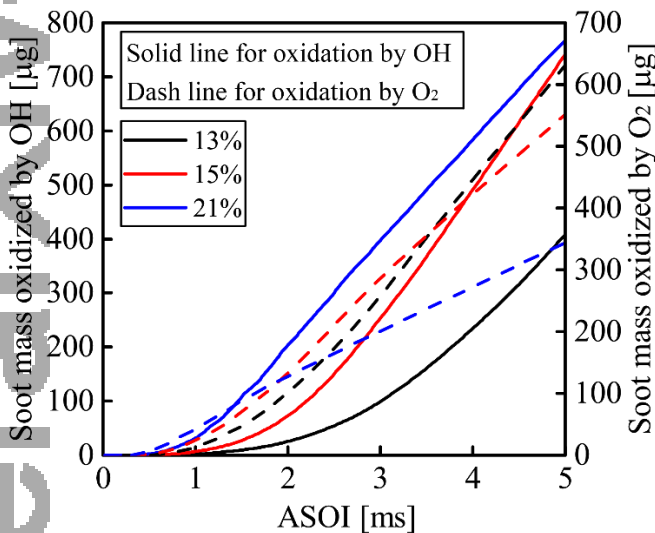


Fig 6 The evolution of soot mass oxidized by OH and O_2 under different EGR levels.

surface after 2 ms ASOI. This leads to a lower oxidation rate by O_2 for 21% O_2 after 2 ms ASOI, although O_2 concentration in 21% O_2 case is higher than other two cases.

3.3 Conclusion

In the present study, soot formation and oxidation processes under different exhaust gas recirculation (EGR) levels are investigated using a phenomenological soot model. The variation of total soot mass with EGR in a monotonic manner is captured by the numerical setup at the ambient temperature of 1100 K. One key point from the analysis is that oxidation, particularly the oxidation by hydroxyl radicals (OH), plays an important role on determining total soot mass, while soot inception and surface growth have less effect on it. At O_2 levels of 15% and lower, the soot number contributed by inception and coagulation does not affect the effective soot surface area significantly, although it is very important for cases at ambient temperature (T_{am}) of 1000 K.

ACKNOWLEDGEMENT

Min Zhang was sponsored by China Scholarship Council (CSC). The computations were performed using the Niflheim cluster at Technical University of Denmark (DTU).

REFERENCE

- [1] Idicheria CA, Pickett LM. Soot formation in diesel combustion under high-EGR conditions. SAE Tans 2005; 114:1559-74.
- [2] Farrace D, Bolla M, Wright YM, Boulouchos K. Numerical study of the influence of EGR on in-cylinder soot characteristics in a heavy-duty diesel engine using CMC. SAE Trans 2014; 7: 256-68.
- [3] Bi X, Liu H, Huo M, Shen C, Qiao X, Lee CFF. Experimental and numerical study on soot formation and oxidation by using diesel fuel in constant volume chamber with various ambient oxygen concentrations. Energy conversion and management 2014; 84: 152-63.
- [4] Skeen S A, Manin J, Dalen K, Pickett LM. Extinction-based imaging of soot processes over a range of diesel operating condition. 8th US National combustion meeting 2013; 1-13.
- [5] Wang H, Ra Y, Jia M, Reitz RD. Development of a reduced n-dodecane-PAH mechanism and its application for n-dodecane soot predictions. Fuel, 2014; 136: 25-36.
- [6] Pang K M, Jangi M, Bai X S, Schramm J. Evaluation and optimisation of phenomenological multi-step soot model for spray combustion under diesel engine-like operating

conditions. Combust. Theo. and Model, 2015; 19: 279-308.

[7] ECN Spray A. <https://ecn.sandia.gov>. Combust. 2020;

[8] Ranz W E, Marshall W R. Evaporation from drops. Chem. eng. prog, 1952; 48: 141-46.

[9] Reitz RD, Diwakar R. Effect of drop breakup on fuel sprays. SAE Tans, 1986; 218-227.

[10] Shih T H, Liou WW, Shabbir A, Yang Z, Zhu J. A new k- ϵ eddy viscosity model for high reynolds number turbulent flows. Computers & fluids, 1995; 24: 227-238.

[11] Jangi M, Bai XS. Multidimensional chemistry coordinate mapping approach for combustion modelling with finite-rate chemistry. Combust. Theo. and Model, 2012; 16: 1109-32.

[12] Yao T, Pei Y, Zhong B J, Som S, Lu T, Luo KH. A compact skeletal mechanism for n-dodecane with optimized semi-global low-temperature chemistry for diesel engine simulations. Fuel, 2017; 191: 339-49.

[13] Payri R, Viera J P, Gopalakrishnan V, Szymkowicz PG. The effect of nozzle geometry over the evaporative spray formation for three different fuels. Fuel, 2017; 188: 645-60.

[14] Pickett LM, Manin J, Genzale CL, Dennis LS, Mark PB. Relationship between diesel fuel spray vapor penetration/dispersion and local fuel mixture fraction. SAE Trans, 2011; 4: 764-99.

[15] Pei Y, Hawkes ER, Kook S. A comprehensive study of effects of mixing and chemical kinetic models on predictions of n-heptane jet ignitions with the PDF method. Flow, turbu. combust. 2013; 91: 249-80.