

## A NUMERICAL STUDY OF NO AND SOOT FORMATION IN AN AUTOMOTIVE DIESEL ENGINE FUELED WITH DIESEL-B ODIESEL BLENDS

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### Abstract

In this paper, engine simulation results are presented to give information on the effect of diesel-biodiesel blends on combustion and emission characteristics of a multiple injection automotive diesel engine. Numerical Study was performed in Computational Fluid Dynamics (CFD) simulation software AVL-FIRE coupled to AVL-ESE Diesel. An improved version of the ECFM-3Z combustion model has been applied coupled with advanced Zeldovich and Kinetic models for NO and soot formation, respectively. The simulation results were validated against the experimental results by comparing the in-cylinder pressure and heat release rate for diesel-biodiesel blends at 2000 rpm under 100% load, and a maximum variation of 5% deviation on the peak cylinder pressure and 4% for heat release rate was found. Simulation results revealed that with the increase of biodiesel amount in the fuel, CO and soot emissions were reduced while NO increased at the simulated operating conditions. In addition, in-cylinder NO and Soot mass fractions were found to be high at 20 and 10 CA ATDC, respectively.

**Keywords:** Diesel Combustion, Biodiesel, NO and Soot Formation

### 1. Introduction

Biodiesel is a notable alternative to petroleum diesel, which should conform to international standards such as ASTM D6751 and EN 14214 specifications for use in diesel engines when it is produced from vegetable oils and animal fats by transesterification. The European Commission set the target to replace 10% of the energy used in transportation with biofuels by 2020 [1], and a large portion of biofuel use is expected to be biodiesel. Accordingly, its production and use probably increases in the next years. Previous researches with biodiesel fuels from vegetable oils [2] and with some others made using unconventional feedstocks [3][4], have demonstrated advantages on diesel emissions such as hydrocarbon (HC), carbon monoxide (CO), and PM but generating higher NO<sub>x</sub> emissions [5][6] when combusted in diesel engines. In addition, it is a renewable, biodegradable, non-toxic and engine-friendly (due to its excellent lubricity) alternative fuel. Although numerous experimental studies have been conducted on biodiesel use in diesel engines, in recent years, researchers have turned their interest on numerical simulations using CFD tools [7], as experimental testing is usually costly and time-consuming [8]. In addition, numerical simulations allow a better understanding of the in-cylinder phenomena. An et al. [9] studied the impacts of biodiesel blend ratio on the emission formation processes of a diesel engine using 3-D CFD simulation software KIVA4 coupled with CHEMKIN II. Yuan et al. [10] developed a detailed numerical spray atomization, ignition, and combustion model using KIVA3V code for investigating NO<sub>x</sub> emissions. The effect of the fuel

temperature on the combustion and emissions characteristics is investigated numerically by Ren and Li [11]. The effect of different injection strategies on the pollutant formation were studied by Meloni and Naso [12] and Wang et al. [13] while Som and Longman [14] investigated the influence of fuel properties on the combustion and emission characteristics of the compression ignition engine focusing on the spray behavior.

In this study, the combustion and emission characteristics of an multiple injection automotive diesel engine fueled with diesel-biodiesel blends was simulated by using a computational fluid dynamics (CFD) software AVL-FIRE, and the results were validated against the experimental results acquired on an engine test-bed. A diesel fuel (B0) and the blends of diesel with biodiesel (soybean oil based) in percentages of 10% (v/v) (B10), 20% (v/v) (B20) and 30% (v/v) (B30) were employed as test fuels at a constant speed of 2000 rpm under full load condition.

### 2. Numerical Study

Numerical study was conducted using 3D CFD software AVL-Fire, which is thermo-fluid dynamics software, and it uses a pressure based segregated solution algorithm. AVL-ESE Diesel, which is a part of the AVL-Fire package, was used to set up, simulate, analyze and optimize aerodynamics, fuel injection, and combustion and emission formation in Diesel engines [15]. The engine specifications, initial and boundary conditions and sub-models employed are given in Tables 1, 2 and 3, respectively.

**Table 1 Engine Specifications**

maximum power	75 kW @ 4000 rpm
maximum torque	280 Nm @ 2000 rpm
cylinder arrangement	four cylinders, in-line
bore (mm)	82
stroke (mm)	90.4
compression ratio	18:1
displacement (L)	1.9
fuel injection	common rail, with pilot
number of nozzle holes	6
spray angle	140°
nozzle hole diameter	0.145mm

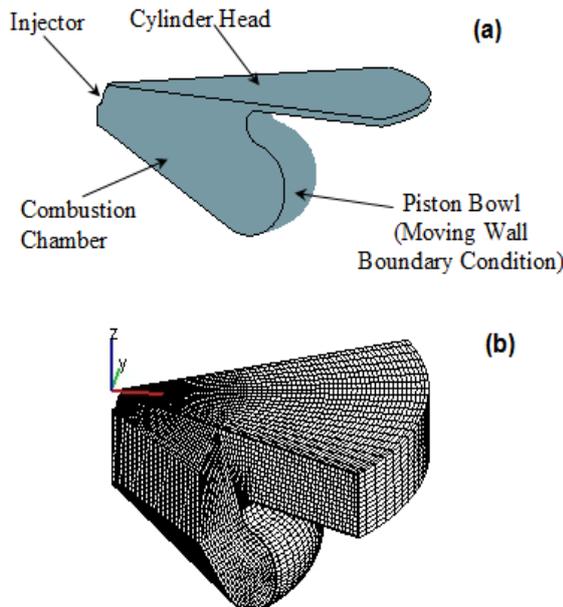
**Table 2. Initial and boundary conditions**

Engine speed	2000 rpm
Intake air temperature	293.15 K
Intake air pressure	1.4 bar
Fuel injection temperature	320.15 K
Cylinder head temperature	550.15 K
Piston top temperature	550.15 K
Cylinder wall temperature	470.15 K
1. Start and end of injection	-20/-10 CA
2. Start and end of injection	5 / 15 CA
Fuel consumption rate	5.8

**Table 3. AVL-FIRE Sub-Models**

Spray Model	WAVE
Spray Wall Interaction Model	Walljet
Droplet Evaporation Model	Dukowicz
Combustion model	ECFM-3Z
Turbulence model	k-zeta-f
Ignition model	Auto-Ignition
NO formation	Extended Zeldovich Mechanism
Soot formation	Kinetic

A three-dimensional mesh of engine combustion chamber was built based on the basis of the engine piston geometry (**Figure 1**). Computations are performed on  $60^\circ$  sector meshes with approximately 100000 cells near at TDC.

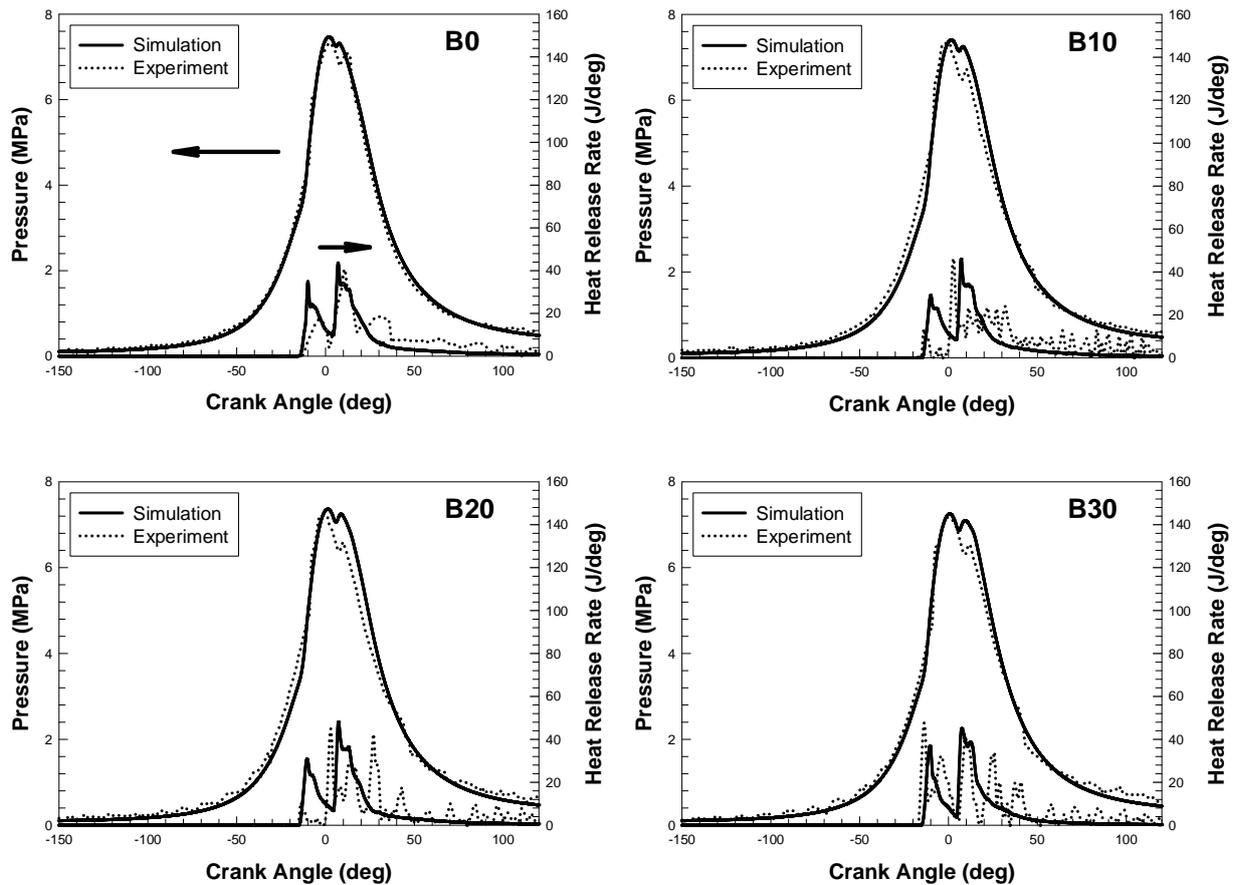
**Figure 1** Computational domain

The experimental tests were carried out in a four-cylinder, four-stroke, turbocharged, direct-injection,

1.9 L Fiat diesel engine coupled to a hydraulic brake. Engine tests were carried out at 1000, 2000 and 3000 rpm under full throttle position. The cylinder pressure signal was determined by averaging 200 pressure cycles obtained with a fiber optic pressure sensor Optrand D33288-GPA (with a sensibility of 1.35mV/psi). A zero-dimensional thermodynamic model was used to determine the main parameters of the combustion process, such as the heat release rate (HRR).

### 3. Model validation

The simulation results were compared with those obtained from experimental testing in **Figure 2**, which was carried out at 2000 rpm. Validation was made by comparing the in-cylinder pressure and heat release rate for B0, B10, B20 and B30 fuels. The first peak cylinder pressure of 7.31 MPa, 7.33 MPa, 7.23 MPa and 7.17 MPa for B0, B10, B20 and B30, respectively, was obtained from experimental testing while in the case of simulation they were 7.46 MPa, 7.39 MPa, 7.36 MPa and 7.25 MPa. On the other hand, the experimental second peak pressure is lower than those obtained from simulation. The maximum deviation in the peak cylinder pressure was found to be less than 5%. For HRR, a similar trend is seen from the figure, the difference does not exceed 4%. Simulated HRR values are in advance compared with experimental ones especially in case where first injection occurred except for B30 [16].



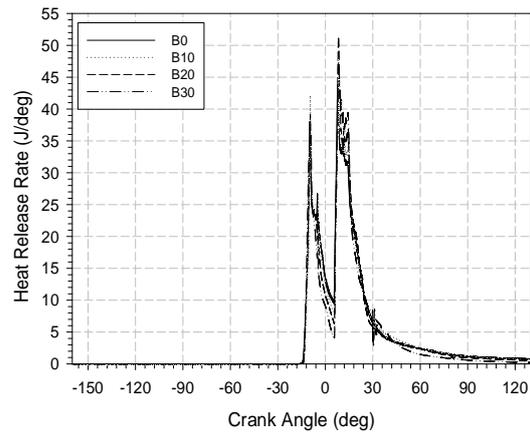
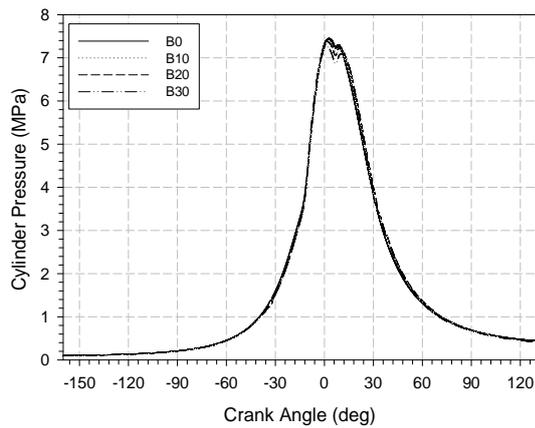
**Figure 2** Experimental and calculated in-cylinder pressure and heat release rates with respect to mixing ratios of biodiesel

## 5. Results and discussions

### 5.1. Combustion characteristics

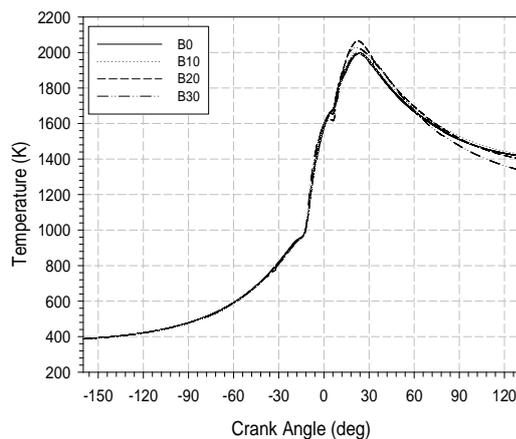
The change in cylinder pressure and heat release rate for diesel-biodiesel blends is shown in **Fig. 3**. The cylinder peak pressure is highest with diesel followed by B10, B20, B30, and these differences are respectively of 0.0418 MPa, 0.0817 MPa and 0.2076 MPa according to the corresponding biodiesel amount in the fuel. In case of the first injection, the maximum pressure for all fuels occurs within the range of 0-5 CA ATDC while for second it is within 7-12 CA ATDC. In HRR graph, two curves are seen;

the first one corresponds to the pre-injection while the second (the larger one) is the main injection, and they have very similar trend for all of the fuels. However, at around the TDC, a lower HR is appeared for blended fuels. The combustion advance reported in the literature [16] for biodiesel fuels is not high enough for present study. **Lapuerta et al.** [17] reported that in multiple injection common-rail engines, the cetane number is the main property responsible for differences in combustion timing whereas this effect is negligible as biodiesel content in the fuel is relatively low.



**Figure 3** Comparison of (a) the in-cylinder pressure, and (b) the heat release rate (HRR) for diesel-biodiesel blends

**Figure 4** shows in-cylinder average combustion temperature against crank angle diagrams for the fuels. The average combustion temperature starts to increase rapidly after the pilot injection where the ignition is started, and reaches to its first peak value for a slightly higher than 1600 K for each fuels, as shown in **Fig. 4**. The second peak, the highest one, was occurred after 21 CA ATDC, and in this case the temperatures above 2000 K were obtained with biodiesel blended fuels while it was 1990 K for diesel case. The highest NO formation was also observed in these conditions for blended fuels. It can already be seen that the regions with higher NO concentrations matched very well with higher temperature zones (this will be discussed later). On the other hand, the pilot injection reduces the ignition delay and therefore the amount of premixed combustion, leading to lower temperatures.

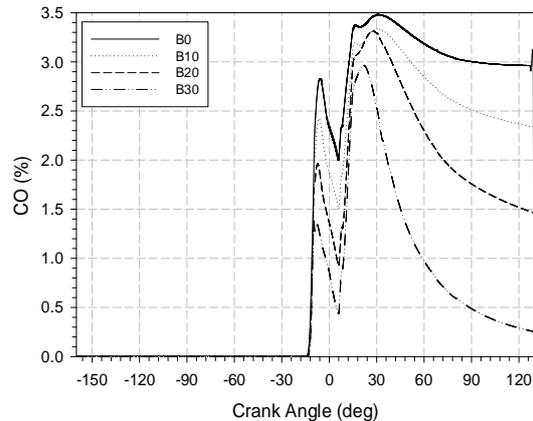


**Figure 4** In-cylinder average combustion temperature for fuels

**5.2. Emission characteristics**

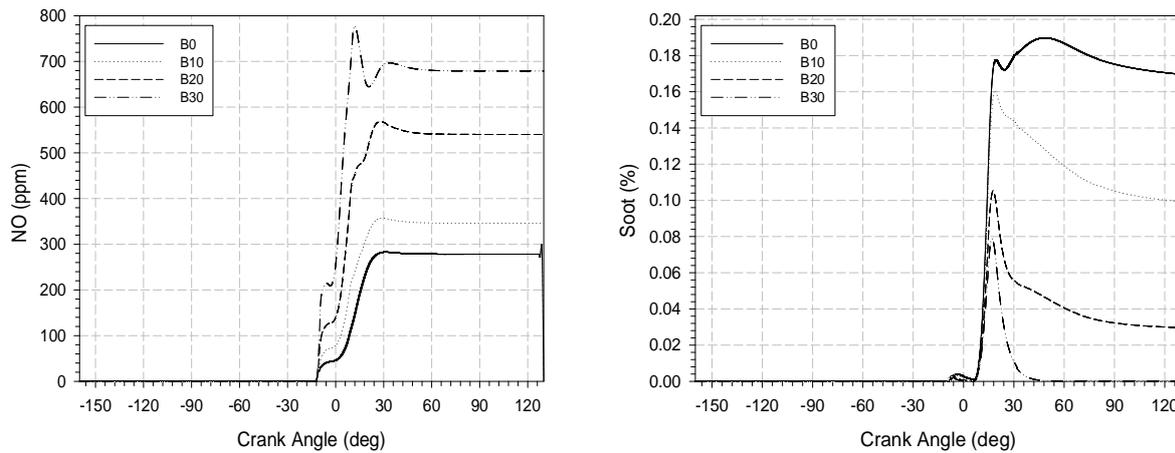
The temporal development of the CO for tested fuels is shown in **Fig. 5**. The CO starts to form before TDC when the pilot injection was occurred, and then CO

formation was increased as the main injection was made at ATDC. On the other hand, the peak in-cylinder CO concentration was found to be the greatest for diesel fuel, and it was reduced with the increase of biodiesel ratio in the fuel, which is attributed to the oxygen content in the biodiesel contributing to more complete combustion [17].



**Figure 5** In-cylinder CO emission histories with respect to crank angle for diesel-biodiesel blends

Increase in the emission of NO was observed in comparison with diesel for all biodiesel blends, and the magnitude of this increase depended upon the biodiesel content in the fuel blends, as shown in **Fig. 6-a** where NO is seen as higher at ATDC when the main injection was made for all fuels. It is likely that higher in-cylinder temperature for biodiesel blends than diesel operation, which can be seen in **Fig. 4**, is responsible for NO increase. The soot emissions for the blends are significantly lower than those obtained with the diesel, as shown in **Fig. 6-b**. This reflects the potential of biodiesel blends to reduce soot emissions with respect to the diesel, as it is reported by other authors, and this is mainly due to the oxygen content of the biodiesel fuel molecules.



**Figure 6** In-cylinder emission histories with respect to crank angle (a) NO emissions, and (b) Soot emissions for diesel-biodiesel blends

Local temperature, NO and soot emissions with various biodiesel ratios are shown in **Fig. 7-8**. Obviously, higher biodiesel ratio leads to higher burned gas temperature, which cause a slightly rise in NO emissions for all three cases. NO may increase due to higher oxygen content of biodiesel blends. The main cause is that biodiesel have higher viscosity hence the droplet size after start of injection is estimated to be larger than that of diesel fuel. These fuel droplets have all combustion process and important heat release rate during the late combustion process. The soot emissions are another important parameter used to appraise the combustion characteristics of test fuels. Soot is usually formed in the overly fuel rich regions in cylinder. Indeed, the high soot concentration areas move in the direction to the piston bowl wall in biodiesel blends as the flame propagation. **Fig. 7-8 (right)** shows the variation of local soot mass fraction of diesel and biodiesel blend fuels with depend on crank angle. It is observed that the use of biodiesel blends improve the combustion process and reduces the soot emissions. Therefore these results confirm the combustion and temperature data.

### Conclusion

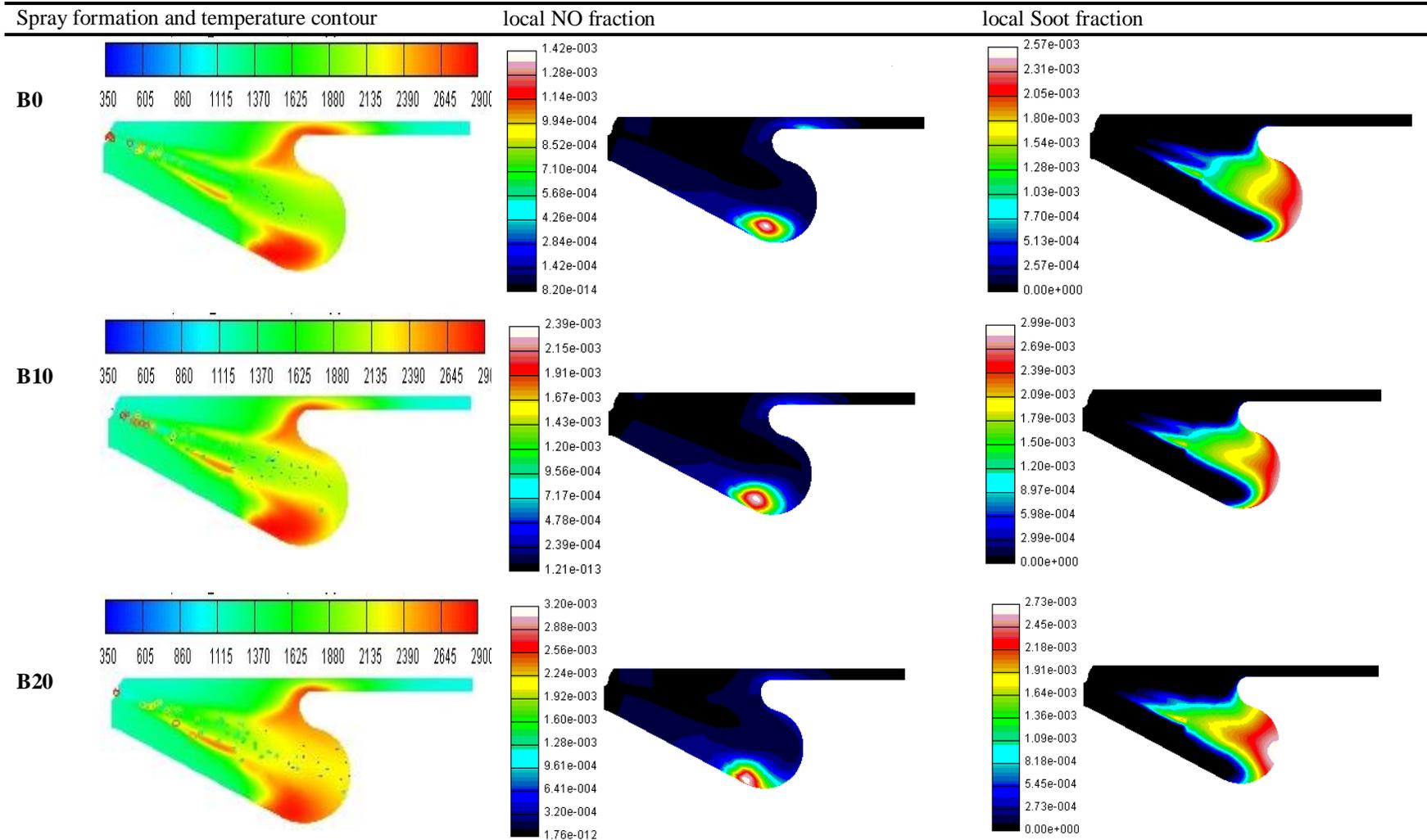
In this study, the authors have investigated the performance, combustion and emission characteristics of diesel fuel and biodiesel blends in a direct injection diesel engine at multiple injection case. Model validation was performed for the AVL-FIRE model in terms of heat release rate and combustion pressure against measurements in the test engine. The conclusions from the results are summarized as the following:

- i. Multi-component combustion model was used of simulation biodiesel combustion for diesel-biodiesel blends and better performance of the results compared to the experimental data.

- ii. Biodiesel blends were presented different combustion characteristics at different engine speed. The peak cylinder pressure and heat release rate were larger at high engine speed.
- iii. Biodiesel blends increased CO<sub>2</sub> and NO emissions at all crank angle while its decreasing CO and soot emission at all crank angle, compared with diesel fuel.
- iv. The combustion and flame temperature increases with the biodiesel blend ratio as slightly.

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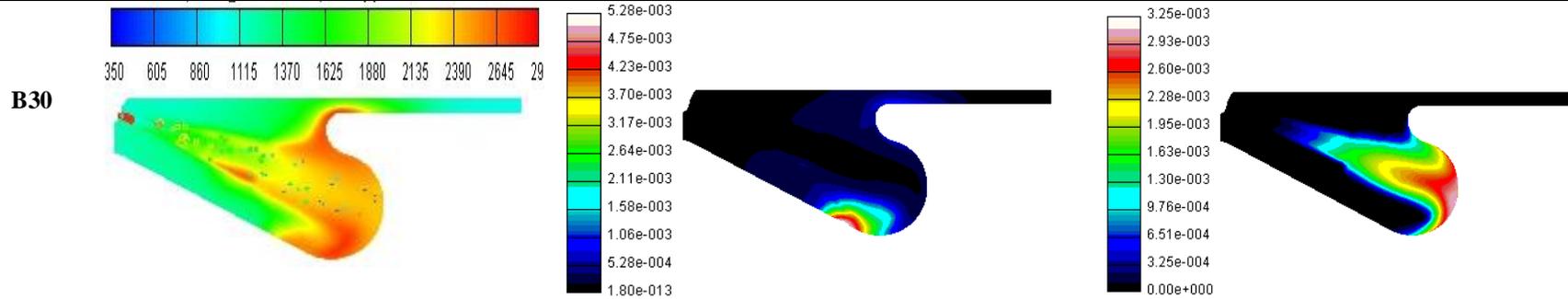
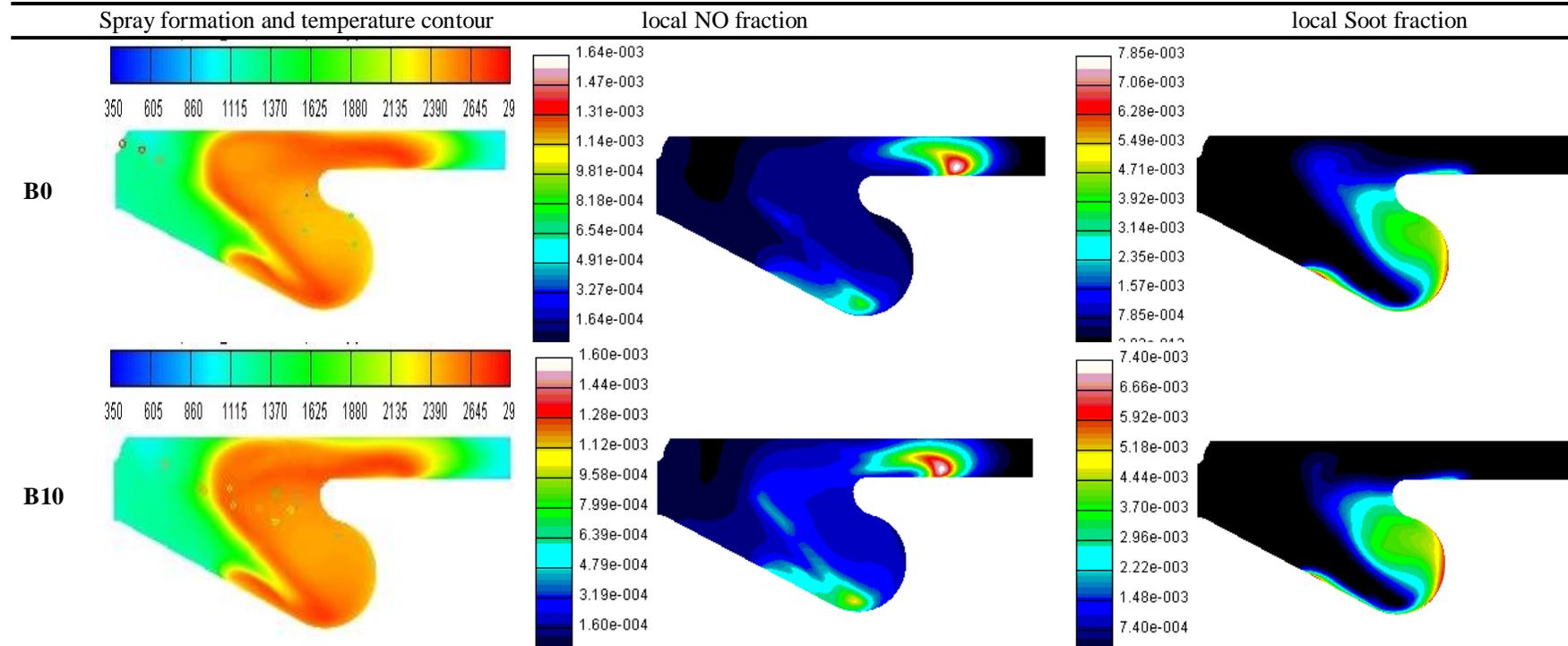


Figure 7 Variation of temperatures, NO and Soot fraction at 10 CA



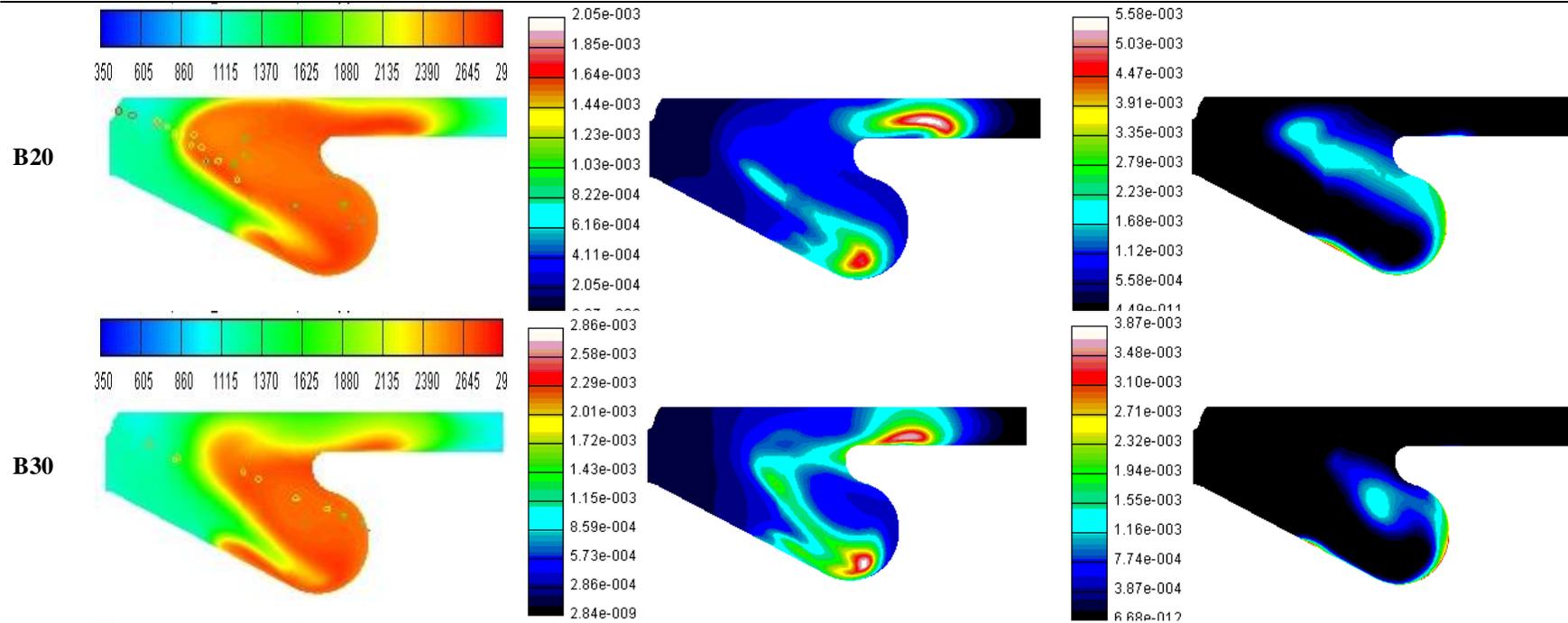


Figure 8 Variation of temperatures, NO and Soot fraction at 20 CA

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