

## MODELING OF CO-COMBUSTION OF BUTANOL WITH DIESEL FUEL IN A DUAL-FUEL COMPRESSION IGNITION ENGINE

*Arkadiusz Jamrozik, Wojciech Tutak*

*Department of Thermal Machinery, Czestochowa University of Technology  
Czestochowa, Poland*

*arkadiusz.jamrozik@pcz.pl, wojciech.tutak@pcz.pl*

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**Abstract.** New challenges posed to internal combustion engines require a fresh approach and the application of modern simulation methods. This study focuses on the numerical analysis of the co-combustion process of diesel fuel with butyl alcohol in a dual-fuel, self-ignition internal combustion engine based on a three-dimensional engine model developed in AVL Fire software. The influence of butanol content, ranging from 0 to 60 %, on engine performance and emissions was investigated. Increasing the amount of butyl alcohol burned with diesel fuel leads to a delay in ignition, decreases maximum cylinder pressure and temperature, and increases the rate of pressure rise and heat release rate. For alcohol content of 20 % and 40 %, there is an increase in pressure and indicated power compared to diesel fuel alone. The addition of butanol to diesel fuel reduces the specific emissions of nitrogen oxides and Soot in the dual-fuel engine. The most favorable case was with a 40 % butanol content. For DB40, the highest IMEP (0.69 MPa) and  $N_i$  (10.37 kW) values were obtained, along with the highest TE efficiency (43.64 %). In comparison to D100, lower NO and Soot emissions were achieved for this case by 35 % and 65 % respectively.

**MSC 2010:** 80A25, 65D17, 68U20

**Keywords:** CFD modeling, n-butanol, dual-fuel diesel engine, combustion, NO emission, Soot emission

### 1. Introduction

In recent years, the internal combustion engine has found application in industry for powering mobile machinery and equipment, as well as in the energy sector for electricity generation in distributed energy systems. Emissions from internal combustion engines can be reduced in various ways. One of them is the use of alternative fuels, which, when derived from renewable sources, emit harmful compounds to a lesser extent during combustion [1]. In industry, the most commonly used type of internal combustion engine is the compression ignition engine, traditionally powered by diesel fuel, in which, due to the ignition characteristics, the use of alternative fuels is difficult. An effective method of burning alternative fuel in a compression ignition

engine is its co-combustion with diesel fuel in a dual-fuel engine [2, 3]. Such an engine has two fuel supply systems: one is the factory injection system for the reactive fuel, which is diesel fuel, and the other is the alternative fuel supply system, with low reactivity, delivered to the intake manifold or directly injected into the cylinder. The ignition source in such an engine is a small dose of diesel fuel, which undergoes autoignition in the cylinder and initiates the ignition of the alternative fuel-air mixture, which would not normally autoignite [4, 5]. One of the research tools increasingly utilized in the analysis of processes constituting the working cycle of a piston engine is Computational Fluid Dynamics (CFD) mathematical modeling [6]. The advancement of numerical modeling is made possible by the increasing computational power of computers, enabling modeling not only of flow processes but also combustion processes in a 3D system [7, 8]. One of the more advanced numerical codes dedicated to modeling the piston engine cycle is the AVL Fire program developed by AVL List GmbH [9, 10]. Khatamnejad et al. [11] conducted research on the co-combustion of diesel fuel with natural gas in a compression ignition engine. The results showed that dual-fuel combustion reduces nitrogen oxides ( $\text{NO}_x$ ) emissions but is associated with higher carbon monoxide (CO) and unburned hydrocarbons (HC) emissions compared to conventional diesel mode. Pham et al. [12] conducted research on the co-combustion of diesel fuel with natural gas in a dual-fuel compression ignition engine. Using the AVL Fire, three-dimensional simulations of the combustion process and emissions were conducted. The simulation results demonstrated that compared to the diesel engine, the dual-fuel engine allows for reducing peak cylinder pressure and temperature values, as well as decreasing emissions of NO, Soot, CO, and  $\text{CO}_2$ . Stipic et al. [13] focused on optimizing the combustion modeling process in a dual-fuel compression ignition engine fueled by diesel fuel and methane. Pressure diagrams in the cylinder and heat release rate obtained from the simulations showed good agreement with experimental measurements, confirming the accuracy and reliability of the modeling approach. Kapusta and Teodorczyk [14] modeled combustion in a dual-fuel engine with direct injection of diesel fuel and propane into the cylinder using AVL Fire. It was found that the dual-fuel mode, compared to the single-fuel mode, led to an increase in peak pressure while simultaneously prolonging the combustion process, more intense formation of NO, and a decrease in fuel conversion efficiency. Pietrykowski et al. in their work [15], presented the results of research on a 3D dual-fuel diesel engine model using AVL Fire software. An analysis of the mixture formation process in engines powered by both indirect and direct methane injection was conducted. For direct injection, a good stratification of the air-fuel mixture was achieved. This created favorable conditions for rapid combustion of the entire fuel dose and reduced the risk of unburned hydrocarbon formation. The objective of this study was to investigate and analyze the co-combustion process of fuels with different physicochemical properties in a compression ignition internal combustion engine based on a 3D engine model developed in AVL Fire software. The analysis focused on the co-combustion process of diesel fuel with butyl alcohol (butanol), where the energy share of butanol in the fuel supplied to the engine ranged from 0% to 60%.

## 2. AVL Fire software

The AVL Fire program enables modeling of thermo-fluid processes in the intake and exhaust manifold as well as in the combustion chamber of a piston engine. This program allows for the calculation of transport phenomena, mixing, ignition, and turbulent combustion in an internal combustion piston engine. It can model both homogeneous mixtures prepared in the combustion chamber and heterogeneous mixtures formed by fuel injection into the chamber. Additionally, calculations can involve either spark-ignition engines [16, 17] or diesel engines [9]. In AVL Fire, the kinetics of chemical phenomena are described by combustion models that account for oxidation processes at high temperatures. The program enables the creation of a three-dimensional computational grid of the engine's computational domain, including intake and exhaust channels, with consideration of valve timing and charge exchange processes. The AVL CFD model is based on solving the equations of conservation of mass, momentum, energy, and quantities of ingredients, which describe the unsteady, three-dimensional flow field. These equations are the three-dimensional Navier-Stokes equations for the compressible fluid mixture [9]. The conservation law can be written:

$$\rho \frac{D\varphi}{Dt} = \rho \frac{\partial \varphi}{\partial t} + \rho U_j \frac{\partial \varphi}{\partial x_j} = \rho \dot{\gamma}_m + \frac{\partial \dot{\gamma}_A}{\partial x_j} \quad (1)$$

where  $\varphi$  is the corresponding property,  $\dot{\gamma}_m$  is an internal source per unit mass of heat due to chemical reaction,  $\dot{\gamma}_A$  is the diffusion flux of heat through the control surface in the energy equation and the force on elementary control surface due to pressure and viscous stresses in the momentum equation,  $\rho$  is fluid density,  $U$  is velocity,  $x$  is the coordinate. Momentum Equations – Navier-Stokes equations  $\varphi = U_i$ :

$$\rho \frac{DU_i}{Dt} = \rho \frac{\partial U_i}{\partial t} + \rho U_j \frac{\partial U_i}{\partial x_j} = \rho g_i + \frac{\partial \sigma_{ij}}{\partial x_j} = \rho g_i - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[ \mu \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial U_k}{\partial x_k} \delta_{ij} \right) \right] \quad (2)$$

where  $t$  is time,  $\delta_{ij}$  is the unit tensor,  $g_i$  is the specific body force,  $\mu$  is viscosity. Energy equation  $\varphi = H$ :

$$\varphi = H = h + \frac{U^2}{2}$$

$$\rho \frac{DH}{Dt} = \rho \left( \frac{\partial H}{\partial t} + U_j \frac{\partial H}{\partial x_j} \right) = \rho \dot{q}_g + \frac{\partial p}{\partial t} + \frac{\partial}{\partial x_i} (\tau_{ij} U_j) + \frac{\partial}{\partial x_j} \left( \lambda \frac{\partial T}{\partial x_j} \right) \quad (3)$$

where  $\dot{q}_g$  is heat flux. Concentration equation  $\varphi = C$ :

$$\rho \frac{DC}{Dt} = \rho \left( \frac{\partial C}{\partial t} + U_j \frac{\partial C}{\partial x_j} \right) = \rho \dot{r} + \frac{\partial}{\partial x_j} \left( D \frac{\partial C}{\partial x_j} \right) \quad (4)$$

### 3. Object of numerical research

A research engine was developed based on the four-stroke compression ignition engine, which, after structural modifications, thanks to a new fuel supply system, was adapted for dual-fuel operation. This engine is a stationary unit, two-valve, with a horizontal cylinder arrangement, employing a cooling system by evaporation of the water jacket, commonly used in the industry to drive generators, water pumps, and simple agricultural machinery. For dual-fuel mode, it is equipped with an additional supply system for butanol, delivered during the intake stroke to the intake manifold. The engine is designed to operate at a constant rotational speed and constant load. The engine displacement is 1810 cm<sup>3</sup>, and the compression ratio is 20.

### 4. Characteristics of the tested fuels

Diesel fuel is a type of fuel used in compression ignition engines obtained in the distillation processes of crude oil. European standards specify, among other things, the minimum cetane number value of diesel fuel allowed for sale, which is 51. Butanol (C<sub>4</sub>H<sub>9</sub>OH) is one of the potential alternative fuels that can be used to power internal combustion engines. It is a liquid fuel that can be produced from various raw materials, including biomass, such as cellulose and glucose. Butanol has several advantages as an alternative fuel. It can play an important role in the future, particularly in the context of increasing sustainable fuel production and reducing greenhouse gas emissions and other air pollutants. Table 1 presents the main properties of diesel fuel and butanol.

Table 1. Fuel specifications

	Unit	Diesel	Butanol
Cetane number	–	51	25
Lower heating value (LHV)	MJ/kg	42.5	33.1
Latent heat of evaporation (LHE)	kJ/kg	243	581.4
Autoignition temperature	°C	230	343
Oxygen (O <sub>2</sub> ) mass fraction	%	0	21.6

## 5. Model of a dual-fuel engine powered by butanol and diesel fuel

### 5.1. Engine model geometry

Modeling in AVL Fire begins with constructing a three-dimensional computational grid that covers the working spaces of the engine under study. These include the intake channels and the combustion chamber in the cylinder. The computational grid can be generated through surface or volume discretization. In the case of

a four-stroke internal combustion engine, the computational grid generation procedure should be carried out separately for each engine operating phase related to the working strokes (Fig. 1). As a result of these calculations, a grid consisting of approximately 160,000 cells ranging in size from 0.25 mm to 2 mm was selected.

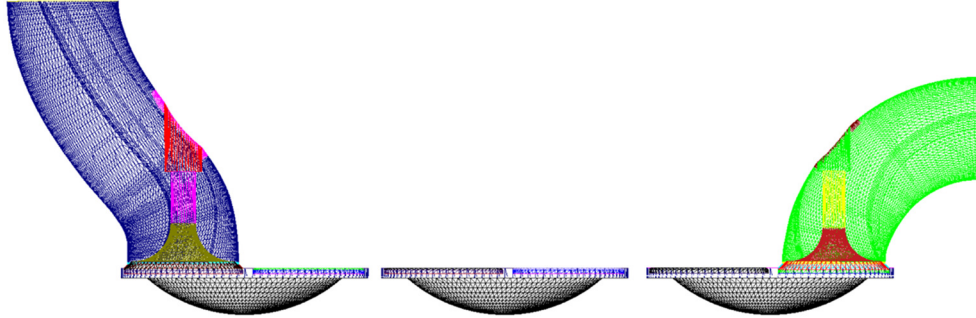


Fig. 1. Computational domains corresponding to the intake, compression, power, and exhaust phases

## 5.2. Initial conditions of the model

To model co-combustion of diesel fuel and butanol in the dual-fuel engine, it was determined that diesel fuel would be supplied to the engine through direct injection into the cylinder (Fig. 2), while butanol would be introduced during the intake stroke as a mixture with air prepared in the intake manifold. An important step in CFD modeling is defining the initial conditions of the model (Table 2).

Table 2. Parameters defining the initial conditions of the process

Parameter	AVL Fire designation	Unit	Value
Fuel mass fraction in the cylinder charge	Fuel mass fraction	–	0-0.0301
Fuel mass	Fuel mass	kg	0-0.0000557
Initial pressure (180 bTDC)	Pressure	Pa	95,000
Initial temperature (180 bTDC)	Temperature	K	340
Turbulence kinetic energy	Turb. kin. energy	m <sup>2</sup> /s <sup>2</sup>	10

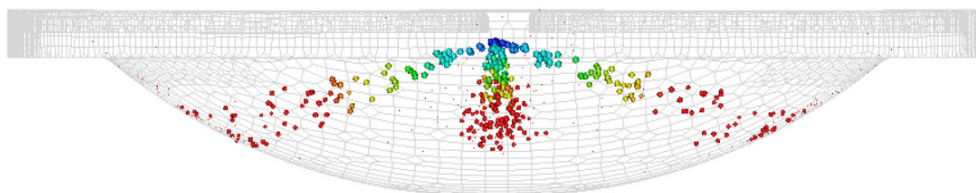


Fig. 2. The shape and direction of the fuel spray (diesel fuel) injected into the combustion chamber of the engine model at 10 deg bTDC

### 5.3. AVL Fire combustion and emission model

Simulations of the combustion process were conducted based on the available Extended Coherent Flame Model, in which turbulent flame in the reaction zone with coherent structure is represented as a collection of elementary laminar flames. Turbulent flow phenomena and heat exchange were computed using the available k-zeta-f turbulence model. The nitrogen oxide formation process was based on the extended Zeldovich model and the Soot formation process on the Lund Flamelet Model [18]. To couple the turbulence with the chemical kinetics, the flame surface density parameter ( $\Sigma$ ) is used, for which an additional transport equation is solved. In general, the average reaction rate is modeled as follows [14]:

$$\bar{\omega} = \dot{\Omega} \cdot \Sigma \quad (5)$$

where  $\dot{\Omega}$  is the local rate of combustion per unit volume.

## 6. Modeling methodology

The modeling was performed on a single computational domain covering the compression stroke and the expansion stroke (from 180 deg before TDC to 180 deg after TDC). At the beginning of the compression stroke, a homogeneous mixture of alcohol and air was present in the cylinder. The first stage of modeling involved compressing this mixture. In the subsequent stage, at the end of the compression stroke, diesel fuel was directly injected into the cylinder. Partial mixing of diesel fuel, alcohol, and air occurred in the cylinder. After the ignition delay period, the resulting mixture underwent auto-ignition, initiating the co-combustion period of diesel fuel with butanol. The modeling considered different energy fractions of butanol in the total energy dose supplied in the fuel to the engine. The combustion process of pure diesel fuel (D100) was investigated first, followed by co-combustion of diesel fuel with 20% (DB20), 30% (DB30), 40% (DB40), and 60% (DB60) energetic fraction of butyl alcohol. The calculations were carried out for a constant energetic dose delivered to the engine.

## 7. Modeling results

The study conducted numerical investigations on the co-combustion of diesel fuel with butyl alcohol based on a model of an engine built in AVL Fire. As a result of the modeling, pressure ( $p$ ) and temperature ( $T$ ) variations in the engine cylinder, heat release rate ( $HRR$ ) profiles, as well as NO and Soot emissions, were obtained. Pressure rise rate ( $PPR$ ) characteristics were determined based on pressure profiles. Total released heat of combustion characteristics were determined based on obtained heat release rates, and by relating them to the maximum value of released heat, normalized heat release ( $Q_{norm}$ ) was obtained.

## 7.1. Combustion characteristics

The primary parameter defining the combustion process in the cylinder of a piston engine is the combustion pressure, determined as a function of volume change or crankshaft rotation angle. Figure 3 illustrates the changes in combustion pressure in the engine cylinder as a function of crankshaft rotation angle during the co-combustion of diesel fuel with butyl alcohol. The highest pressure was obtained during the combustion of pure diesel fuel (8.4 MPa). The addition of butanol resulted in a reduction of the maximum pressure in the cylinder, caused by ignition delay and a shift of combustion after top dead center (TDC). For DB60, ignition of the mixture occurred significantly after TDC, resulting in combustion shifting into the expansion stroke and disturbances in this process evident in the pressure change curve. Temperature variation characteristics during the combustion of diesel fuel and butanol were obtained through modeling. Figure 3 shows temperature profiles, indicating that the addition of alcohol leads to a reduction in the maximum combustion temperature. The highest temperature value in the cylinder, reaching 1773 K, was obtained during combustion of pure diesel fuel.

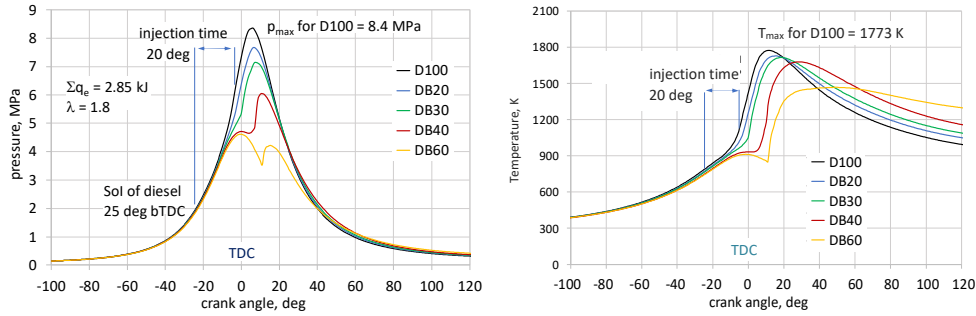


Fig. 3. Pressure and temperature variation curves in the cylinder of the modeled engine

The parameter indicating the nature of the combustion process in a piston engine cylinder is the heat release rate ( $HRR$ ), expressed in J/deg. Heat release rate:

$$HRR = \frac{\kappa}{\kappa-1} p \frac{dV}{d\phi} + \frac{1}{\kappa-1} V \frac{dp}{d\phi} \quad (6)$$

where  $\kappa$  is the ratio of specific heats,  $V$  is cylinder volume, and  $p$  is in the cylinder pressure. Figure 4 illustrates changes in the heat release rate ( $HRR$ ) during combustion in the cylinder of the modeled engine as a function of crankshaft rotation angle. The combustion process of the fuel-air mixture in the cylinder of a piston engine is a complex process consisting of several stages. The most important stages include ignition delay, the diffusive phase determined by fuel spreading, the kinetic phase involving the combustion of the mixed charge, and the burnout phase. In a compression ignition engine, the diffusive phase dominates. Figure 4 shows that in the case of D100, the combustion process has a diffusive nature, and slight ignition delay results in relatively slow combustion. With an increase in the addition of butanol,

ignition delay increases, and the extended time favors mixing of the charge in the cylinder and the formation of a homogeneous mixture. Such a mixture burns rapidly after ignition, increasing the kinetic phase, typical for spark ignition engines. Combustion of DB40 was characterized by the highest  $HRR = 309 \text{ J/deg}$ .

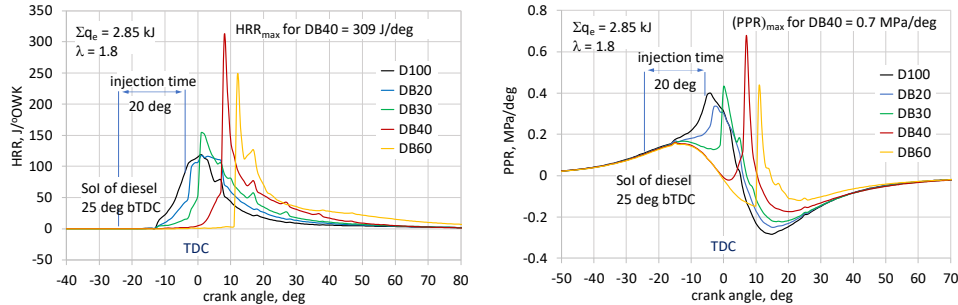


Fig. 4. Heat release rate ( $HRR$ ) and pressure rise rate ( $PPR$ ) curves in the engine cylinder

Figure 4 illustrates changes in the pressure rise rate ( $PPR$ ) as a function of crankshaft rotation angle. The pressure rise rate is a significant indicator of engine performance, especially for a compression ignition engine. An excessively high value of this parameter indicates hard engine work, adversely affecting the crankshaft-piston assembly by increasing its load, and a value exceeding  $1 \text{ MPa/deg}$  may lead to permanent mechanical damage to the engine. From Figure 4, it can be inferred that the engine fueled with DB40 exhibited the hardest work. In this case, the  $PPR$  value of  $0.7 \text{ MPa/deg}$  was higher than that obtained for D100 by approximately  $0.3 \text{ MPa/deg}$ .

As a result of scaling the heat release rate curves, heat release profiles during the combustion process were obtained. Figure 5 presents the released heat normalized to the maximum value. Based on the  $Q_{norm}$  profiles, two main combustion parameters can be determined: ignition delay (ID) and combustion duration (CD). A significant ignition delay in a compression ignition engine is not favorable for its operation. Alcohol fuels such as butanol cause an increase in ignition delay. Combustion duration affects the efficiency of combustion in the cylinder. Intense and short combustion positively impacts the process and leads to increased efficiency.

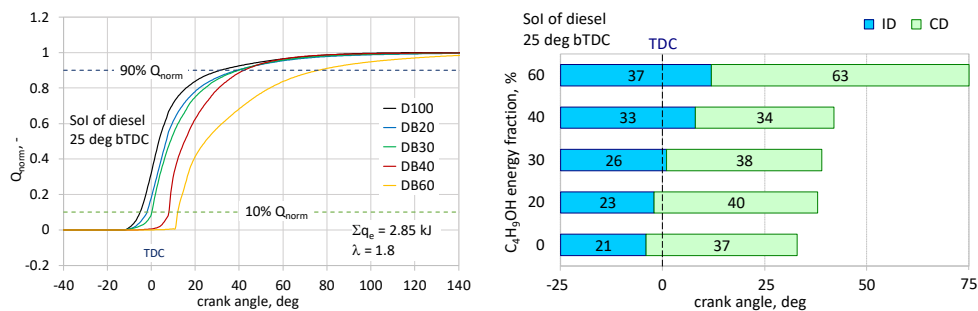


Fig. 5. Heat release and combustion stages in a dual-fuel engine



Figure 5 presents the determined values of ID and CD for pure diesel fuel and for co-combustion of diesel fuel with butanol. The addition of butanol resulted in increased ignition delay compared to D100. For DB30 and DB40, a simultaneous increase in ID and a decrease in CD were observed. The engine co-combusting diesel fuel with 40 % butanol exhibited the shortest CD.

## 7.2. Performance characteristics

The parameters determining the performance of an internal combustion engine are indicated mean effective pressure ( $IMEP$ ) and indicated power ( $N_i$ ). Indicated mean effective pressure:

$$IMEP = \frac{1}{V_d} \oint p dV \quad (7)$$

where  $p$  is in the cylinder pressure,  $V$  is cylinder volume,  $V_d$  is displaced cylinder volume. Figure 6 illustrates changes in the indicated mean effective pressure and thermal efficiency for the analyzed proportions of butyl alcohol. It is evident that with an increase in the alcohol content, both indicated pressure and indicated power rise. However, an exception is observed with the mixture containing 60 % alcohol. The highest indicated pressure and indicated power were achieved during the combustion of diesel fuel with 40 % butyl alcohol content, reaching 0.69 MPa and 10.37 kW, respectively.

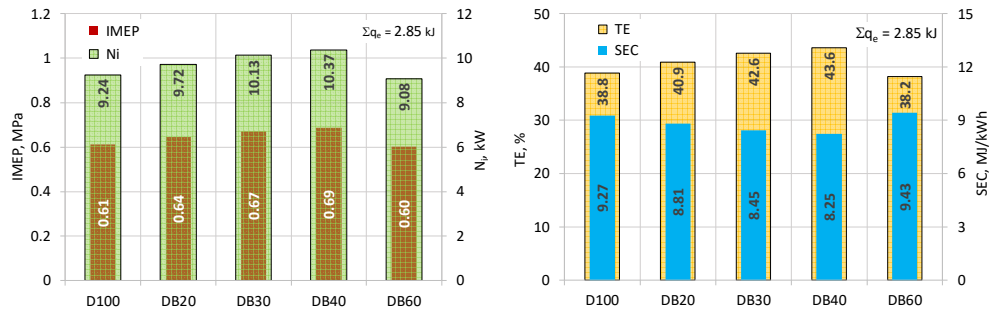


Fig. 6. Indicated mean effective pressure ( $IMEP$ ), indicated power ( $N_i$ ), thermal efficiency ( $TE$ ), and specific energy consumption ( $SEC$ )

The economic aspect of using butanol as a bio-component co-combusted with diesel fuel can be analyzed based on changes in specific energy consumption, expressed in MJ/kWh. In Figure 6, it can be observed that with an increase in efficiency, the specific energy consumption decreases. The addition of alcohol to diesel fuel results in an increase in  $TE$  (thermal efficiency) and a decrease in  $SEC$  (specific energy consumption). The only exception is the mixture containing 60 % alcohol. The highest thermal efficiency was achieved during the combustion of DB40, which was 43.64 %. The specific energy consumption in this case was 8.25 MJ/kWh.

### 7.3. Emission characteristics

#### NO emission

Nitrogen oxides are compounds primarily composed almost exclusively of nitrogen oxide (NO), which forms as a result of the chemical reaction between nitrogen and oxygen during the combustion process in the engine cylinder at high temperatures. Figure 7 presents the calculated emissions of NO and Soot for the dual-fuel engine using butanol/diesel. The emissions obtained from the modeling represent the mass fractions of NO and Soot. To provide a more objective analysis of emissions, the mass fractions were normalized to the indicated power and expressed in g/kWh. It can be observed that the engine with the addition of alcohol exhibited lower specific emissions of NO (except for DB20) compared to D100, resulting from higher combustion temperatures and a faster heat release rate.

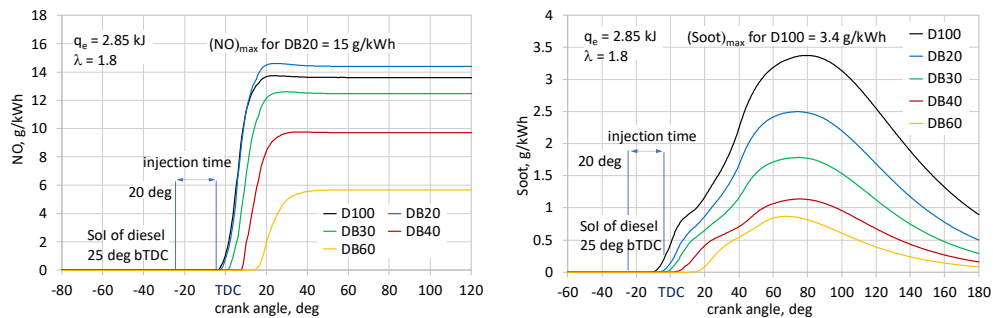


Fig. 7. Specific emissions of NO and Soot

#### Soot emission

Soot is a carbon compound formed during incomplete combustion. Soot is most commonly found in compression ignition engines, where the diffusive phase dominates the combustion process. In Figure 7, it can be seen that the highest amount of Soot is generated in the case of pure diesel fuel. The use of a mixture with alcohol reduces Soot emissions because alcohol contains less elemental carbon compared to diesel fuel. In our case, the additional dose of alcohol is injected into the intake channel, where it vaporizes and forms a homogenous mixture with air, significantly reducing the possibility of fuel-rich zones forming. Additionally, alcohol itself contains oxygen, which participates in combustion and contributes to improving this process.

Figure 8 illustrates cross-sections of the combustion chamber at three piston positions, showing the equivalence ratio (ER, the inverse of the excess air ratio –  $\lambda$ ), temperature, mass concentration of NO, and Soot obtained for DB40. In Figure 8, areas of the combustion chamber where favorable conditions for the formation of nitrogen oxides and Soot exist are depicted. The formation of NO is favored by high temperature and excess air (small values of the equivalence ratio). Soot forms

in regions a with low temperature and in fuel-rich zones (large values of the equivalence ratio).

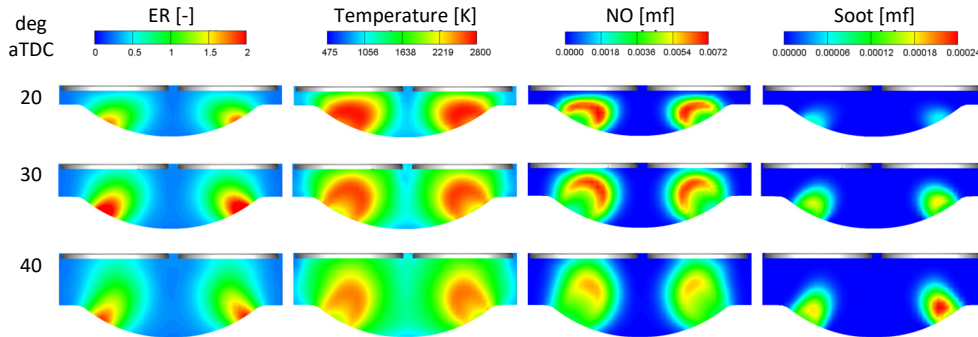


Fig. 8. Spatial-temporal distributions of the ER coefficient, temperature, mass fraction of NO, and Soot at 20, 30 and 40 deg aTDC determined for DB40

## 8. Conclusions

The co-combustion process of diesel fuel with n-butanol was analyzed, with its energy share in the supplied fuel ranging from 0% to 60%. Based on the conducted simulations, it can be concluded that:

- Increasing the amount of n-butanol burned with diesel fuel reduces the  $p_{max}$  and  $T_{max}$  in the cylinder of a dual-fuel engine.
- HRR sharply increases above 20% butanol content. Increasing the amount of alcohol in the cylinder of an engine fueled by butanol and diesel fuel causes a delay in ignition.
- The engine fueled with DB40 is characterized by the shortest CD.
- $IMEP$  and  $N_i$  increase with the rise in alcohol content in the fuel, from 20% to 40%, compared to diesel fuel alone.
- With the increase in alcohol content from 20% to 40% in the fuel, the IE of the engine rises, while the  $SEC$ .
- Increasing the share of butanol above 20% in a dual-fuel CI engine, results in a reduction of NO and Soot concentrations in the engine cylinder.

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