

## The derivation of empirical sub-model for calculation of combustion model parameters

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**Abstract.** In the presented paper the innovative method for derivation of empirical sub-model for calculation of combustion model parameters, when using different fuels or biofuels, is presented.

Combustion model parameters are holding some crucial information about spray development, combustion speed, injection delay, etc.; therefore their accurate determination is necessary if realistic influence of fuel used on combustion process, emission formation process and engine operating characteristics want to be obtained. In previous paper selected L-M optimization method was used for solving the inverse problem of combustion model parameters values determination using pure diesel (D2) and pure biodiesel (B100) fuels. In-cylinder pressure traces are one of the most important engine characteristics; therefore we used experimentally obtained in-cylinder pressure traces as a fitting parameter in objective function of the optimization method. The determined values of combustion model parameters for D2 and B100 were further used when selecting the forms of the sub-model equations. The coefficient of determination  $R^2$  was selected for testing the accuracy of equations using the program for testing the accuracy of different forms of equations made in Mathematica. At the end the accuracy of derived empirical sub-model was tested using D2, B50 and B100 fuels where all the combustion model parameters for numerical simulations were calculated using new derived sub-model. Numerical and experimental results of engine characteristics showed good agreement. This indicate on the possibility of proposed sub-model for accurate determination of mixing controlled combustion model parameters values for numerical testing of diesel engines which are similar to our test engine.

### Introduction

The influence of human development on global pollution is becoming more and more evident. The usages of fossil fuels within the transportation sector extensively contribute to air pollution which is the more evident in city centers where green spaces are lacking. Transportation in the European Union contributes to approximately 21 % of all greenhouse gas emissions. The usage of biofuels can contribute to reductions of greenhouse gas emissions pollution caused by burning the fossil fuels in transportation sector. The production of biofuel can also contribute to the economic development of a country or its region and can help to minimize its dependence on crude oil prices.

Biodiesel fuels also known as methyl esters of vegetable oils are attracting increasing interest. They have low environmental impact compared to fossil fuel and they can be used as an alternative fuels in existing engines. They consumption and production are increasing every year and are stimulated by the raising of crude oil prices, the striving of individual countries to reduce their dependences on imported energy sources, and implementing the Kyoto protocol directives for the reduction of global emissions from greenhouse gasses. [1], [2], [3]

World biodiesel production increased by more than 20 times in 2012 compared to 1990. At the same time ethanol production has increased more than 7-fold. This makes biofuels more accessible for commercial usage and also more attractive. Many EU countries are already mixing biofuels with conventional fuels to meet European Union demand for biofuel usage in transportation sector. [1], [2]

Several experimental and numerical testing should be performed to test how usage of biodiesel fuels influence on engine operating condition and emission formation process before pure biodiesel fuel or its mixtures with commercial fuels can be used in every day transport. Experimental test are very costly and it take a significant amount of time to performed experimental test on several engine operating regimes using different fuels or biofuels. It is because of that that numerical simulation are used when performing parametric studies of biofuels' influences on engines' operating conditions, combustion processes and emissions' formations. Parametric studies are usually made using phenomenological combustion models while complex 3D simulation programs are usually used when analyzing the fuel spray-jet development within a combustion chamber or emission formation zones. The phenomenological combustion models are significantly less time-consuming than 3D simulations and enable us to simulate the whole engine operation under several engine operating conditions which is necessary if we want to numerically perform different engine test-cycles, etc. [4]

Model parameters, commonly used in phenomenological combustion models, are replacing the complex dynamics of air-flow, spray development and emission formation process. They hold some crucial information about spray development process, diffusion combustion speed, injection delay, etc. therefore their accurate determination is necessary. The values of model parameters should be set for each fuel and each engine tested. The values for some parameters for commonly used combustion models and engines types are already known but when a new type of fuel is introduced their determination base on user experience. Therefore, the results from experimental measurements are needed to confirm the results of numerical simulations which also, consequently, confirm the selected values of model parameters. [5]

In the presented paper sub-model for calculation of combustion model parameters was derived. First all combustion model parameters were tested to determine which parameter have influence on numerical results. This test also indicates which parameter we will be able to determine using inverse optimization process. In previous paper [6] selected LM optimization method was used for solving the inverse problem of combustion model parameters values determination using pure diesel and pure biodiesel fuels. The experimentally obtained in-cylinder pressure was used as a fitting parameter in optimization method objective function. The determined values of combustion model parameters were further used for selection of sub-model equation.

### Selection of combustion model parameters used for optimization variables

All AVL MCC combustion model parameters, presented in [7] and [8], can be used as a design variable in inverse optimization process. It is necessary to first perform a test if different values of combustion model parameters have influence on the results of numerical

simulations. If some parameter don't have influence on final numerical results or is its influence small we won't be able to precisely determine parameter value using optimization process and the results of experimental measurement. We must also consider if some parameter can be determined from experimental results without optimization process.

Figure 1 presents the parameter values influence on maximal obtained in-cylinder pressure ( $p_{max}$ ), angle of where maximal pressure occur ( $\alpha_{p_{max}}$ ), engine rated torque (torque), engine rated power (power) and exhaust gas temperature ( $ex\_g\_temp$ ). The presented results show relative difference between the obtained results at parameter value 1 (default value) and all other values. The selected interval was proposed from the developer of AVL BOOST simulation program. When changing the value of one parameter all other parameter values were left on default value 1.

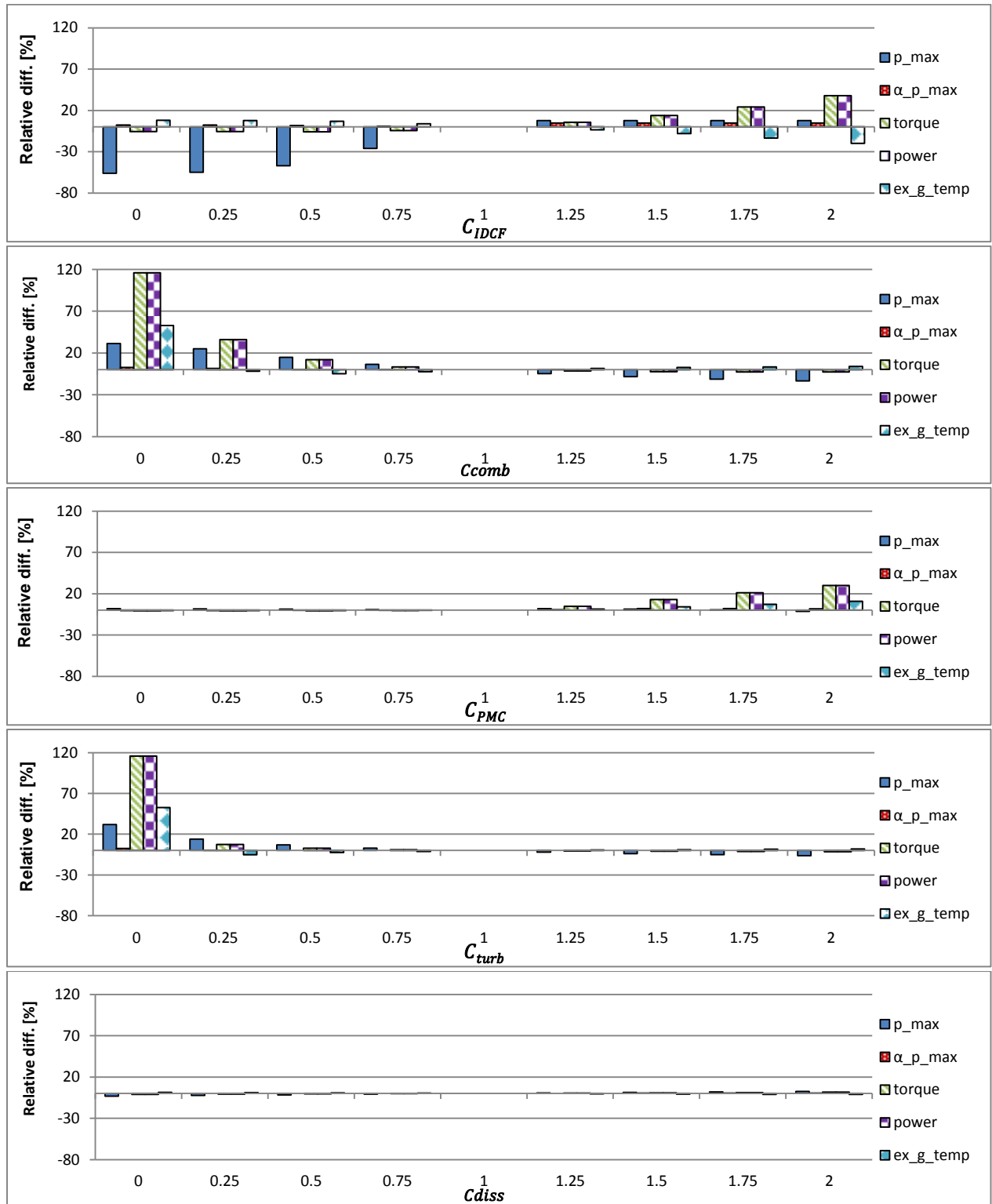


Figure 1: Influence of parameter values on numerical results

From the presented results can be concluded that all parameters, except dissipation parameter,  $C_{diss}$ , have influence on numerical obtained results and can be determined using optimization method. In order to shorten optimization time we have decided to determine the turbulence parameter  $C_{turb}$  using the experimental results of injected fuel mass per cycle. Dissipation parameter will be kept constant on its default value for all fuels on all operating regimes.

### Experimental set-up

The experimental measurements were performed on a 6-cylinder naturally aspirated, four stroke heavy-duty MAN diesel engine. The engine was placed on engine test bed and equipped with all measuring equipment needed. Engine tests were made on 1360, 1700 and 2000 engine speed under full throttle position (full engine load for each fuel). Kistler 6001 piezoelectric pressure transducers was mounted in combustion chamber of first engine cylinder for measuring the in-cylinder pressure trace further used in inverse optimization process.

### Determination of selected combustion model parameters

Selected combustion model parameters  $C_{IDCF}$ ,  $C_{comb}$  and  $C_{PMC}$  were used as a design variable in inverse optimization process. Using the selected L-M optimization method and experimentally obtained in-cylinder pressure all three parameters were determined for pure diesel and pure biodiesel fuel on selected engine operating regimes. All three parameters were determined for one fuel on one engine operating regime simultaneously. The determined values of combustion model parameters for diesel and biodiesel fuel were further used in derivation of sub-model for calculation of combustion model parameters.

### Derivation of sub-model for calculation of combustion model parameters

Sub-model for calculation of combustion model parameters will allow the user to calculate each parameter value base on known fuel properties and engine operating regime. Figure 2 presents the influence of engine speed and fuel properties on parameter value.

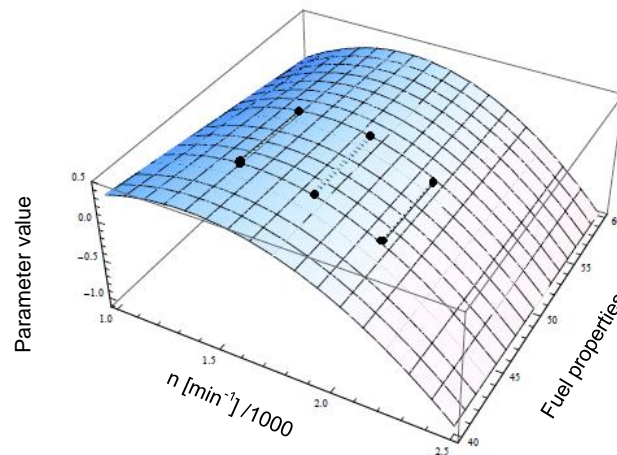


Figure 2: The influence of engine speed and fuel properties on parameter values

It can be seen from Figure 2 that the correlation between combustion model parameter values, engine speed and fuel properties is not linear and that interpolation function will be needed for each parameter to describe its dependency of the engine speed and fuel properties. The forms of the Equations 1 - 3 for determining each parameter value were selected using the values of combustion models' parameters obtained during the inverse optimization process. It was for that purpose that the program for testing the accuracies of different forms of equations was created in Mathematica. The accuracies of several forms of equation were tested using the coefficient of determination  $R^2$ . The calculated values for parameters D2 and B100 were compared to the values for those parameters determined during the inverse optimization process. The  $R^2$  values for the selected equations were greater than 0.99, thus providing good accuracy for the selected equations of the proposed sub-model.

$$C_{IDCF\ i,j} = -0.057931 \cdot e^{n_j} \cdot CN_i + 0.377201 \cdot n_j \cdot CN_i + 6.56338 \cdot n_j^2 - 25.6968 \cdot n_j - 0.326347 \cdot CN_i + 25.1403 \quad (1)$$

$$C_{comb\ i,j} = -0.286503 \cdot e^{n_j} \cdot CV_i + 1.35589 \cdot n_j \cdot CV_i + 74.8476 \cdot n_j^2 - 227.799 \cdot n_j - 0.722727 \cdot CV_i + X_i + 171.666 \quad (2)$$

$$C_{PMC\ i,j} = -0.025944 \cdot n_j \cdot CN_i + 0.0638479 \cdot n_j^2 + 0.933666 \cdot n_j + 0.0335885 \cdot CN_i - 1.10891 \quad (3)$$

The selected equations are just one of the possible forms of equations and do not represent the only possible forms of the equations. In Equation 1 the ignition delay calibration factor  $C_{IDCF}$  was expressed as a function of the fuel cetan number  $CN_i$  and engine speed  $n_j$ . The fuel cetan number defines the ability of the fuel to ignite within compression ignition engines and is a significant indicator of the fuel's quality. Fuels with a better ability for ignition have higher cetan numbers and vice versa. Therefore  $CN_i$  has a greater impact on the ignition delay period,  $C_{IDCF}$  parameter, and also on the amount of fuel mass that will burn in the premixed part of the combustion, as defined by  $C_{PMC}$ . The combustion constant  $C_{comb}$  defines the fuel combustion speed during the diffusion part of the combustion process. Combustion speed is limited by the speed of fuel vapor formation and by the diffusion of air (oxygen) molecules in the combustion front. Combustion speed also influences the shape of the rate regarding the heat release curve, which is influenced by the fuel's calorific value. Both the fuel oxygen content  $X_i$  and the calorific value  $CV_i$ , are included in the equations for calculating the combustion parameter. Equation 1 -3 were used for calculation of all needed combustion model parameter for pure diesel fuel, pure biodiesel fuel and their 50 % mixture B50.

### Results and discussion

Numerical testing of engine characteristics was performed in the presented study using AVL BOOST simulation program and their MCC combustion model. Three combustion model parameters were calculated using the proposed sub-model for their calculation. Other two parameters were determined from experimental results or were kept on their default value.

Experimental and numerical results of engine rated torque, power and brake specific fuel consumption (BSFC) are presented in Figure 3.

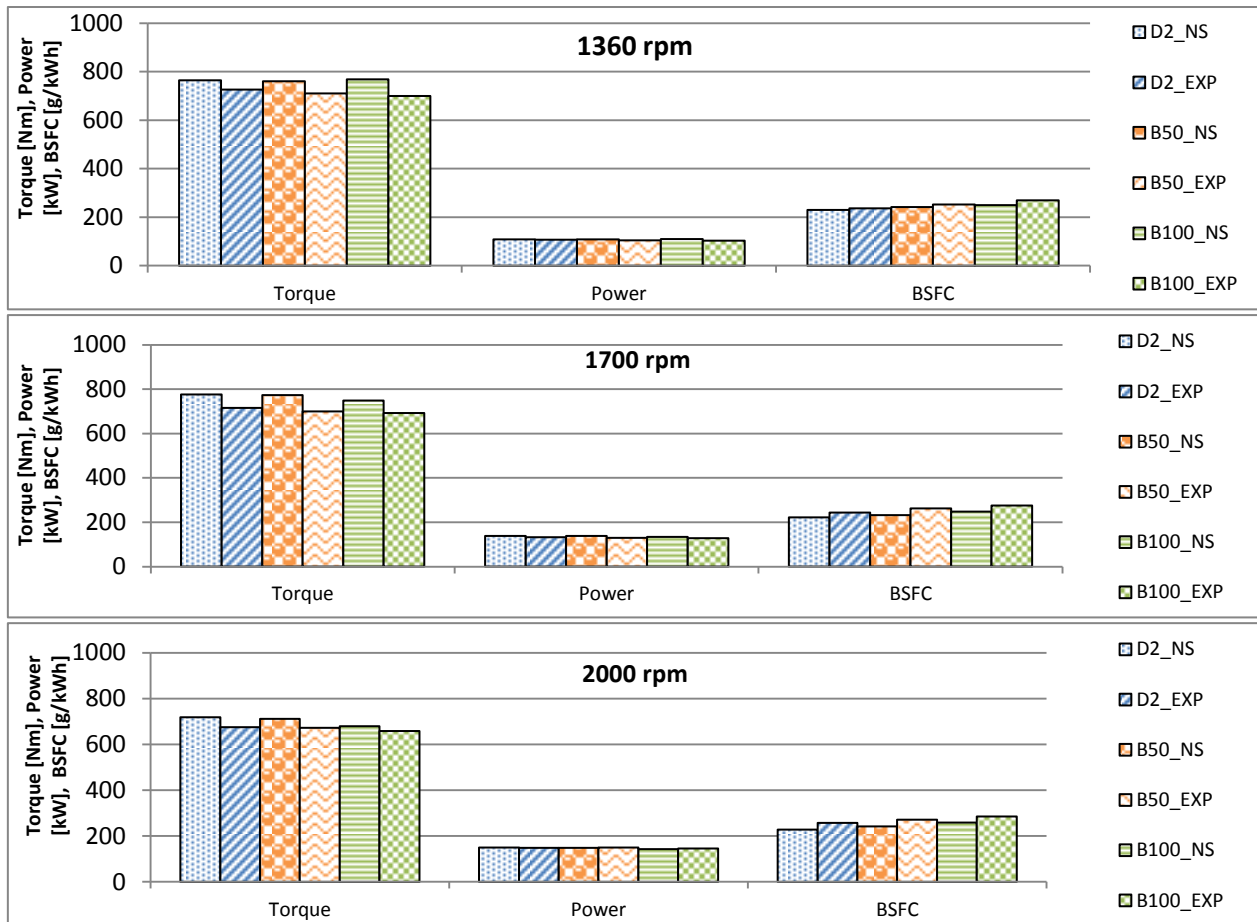


Figure 3: Experimental and numerical results

The experimental and numerical results presented in Figure 3 show good agreement between the numerical and experimental results of engine rated torque, power and BSFC. Experimental results indicate that usage of biodiesel fuel influence on reduction of obtained engine torque and power. Numerical results also indicate on reduction of engine rated power and torque on higher engine speeds while slighter increase of power and torque was obtained on 1360 rpm. Engine rated power and torque are reduced because of lower biodiesel fuel calorific values.

Both, numerical and experimental results indicate on increased brake specific fuel consumption when using biodiesel fuel or its mixtures. The increase in brake specific fuel consumption was also caused by the decrease of biodiesel fuel calorific value.

The comparison between numerical and experimental results is good. Maximal differences are around 6 % which is in common range when comparing numerical and experimental results. This indicates that proposed sub model is suitable for calculation of selected combustion model parameters and can determine their values with reasonable accuracy. It presents a useful tool for determining model parameters based on tested fuel properties and engine operating regimes. For wider usages of the sub-models several different measurements should be performed at different engine speeds and different throttle positions.

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