Usage of optimization methods for determination of combustion model parameters

L. Lešnik[1] and B. Kegl[2]

[1]Luka Lešnik, University of Maribor, Faculty of mechanical engineering, Engine research Laboratory, Smetanova ulica 17, SI-2000 Maribor, Slovenia, luka.lesnik@um.si

[2] Dr. Breda Kegl, University of Maribor, Faculty of mechanical engineering, Engine research Laboratory, Smetanova ulica 17, SI-2000 Maribor, Slovenia

Keywords: AVL MCC combustion model, parameters, optimization methods, AVL BOOST

Abstract. This paper presents an innovative method for determination of combustion model parameters by using optimization methods. The accuracy of combustion models depends highly on proper selection/determination of combustion model parameters. The model parameters of a phenomenological combustion model in an internal combustion engine depend on the engine's design and operating conditions, and need to be determined for each engine type and operating condition separately. These parameters are often determined manually, based on the results of experimental measurements that require several simulation test runs and need to be repeated for every operational regime of the simulated engine and every used fuel or biofuel. The determination of the AVL MCC combustion model parameters in this paper is defined as an inverse problem which is solved by using various optimization methods. Three different optimization methods with different search techniques were tested on one operating regime of the ESC 13 mode test. All the optimization methods were able to determine the combustion model parameters and the obtained results agree well with the experimental results. According to the results, the L-M method was selected as the most promising for further determination of the combustion model parameters. The main advantages of the L-M method are fast convergence (low computation time) and good agreement with the experimental results.

Introduction

Global pollution is becoming more and more apparent throughout the Globe. Scientists are working to reduce the pollution of the Earth as much as possible by reducing energy consumption within all fields of human development. When talking about diesel engines, alternative fuels may offer one solution towards reducing those harmful emissions that are a product of fossil fuel combustion, without affecting engine power and fuel consumption drastically. One of the more promising alternative fuels that could be used in diesel engines is biodiesel fuel, which can be made from different sources of raw materials such as rapeseed oil, canola oil, animal tallow, etc. Different sources of raw materials for biodiesel production would influence the physical and chemical properties of biodiesel. This has resulted in the need for constant investigations about how biodiesel influence a diesel engine's performance and exhaust gas emissions when introducing new types of biodiesel fuels. Over recent years many experimental and numerical investigation have been done in order to confirm the possible usages of different types of biodiesel in diesel engines. Because experimental researches can sometimes be very costly and time-consuming, they are often replaced by using numerical simulations, [1, 2, 3, 4, 5].

When simulating an engine's operations and conditions inside a combustion chamber, we can use more complex, more detailed, and more time-consuming 3D simulations [6], or we can use simpler but still enough accurate thermodynamic and phenomenological combustion models such as the MCC combustion model developed by Chmela and Orthaber [6]. Although a complex 3D combustion model provide use more information about the conditions within the combustion chamber, and spray development [7], thermodynamic and phenomenological combustion models are much more applicable for performing parametric studies into how different engine settings and different fuel characteristics influence engine performance and exhaust gas emissions. Parametric studies can replace time-consuming and expensive experimental measurements, but for performing parametric studies the combustion models' parameters need to be accurately set. The model parameters of a thermodynamic combustion model depend on the internal combustion engine's specifics and engine operating conditions, and need to be determined for each and every engine type and operating condition separately. They are normally determined manually based on the results of experimental measurements that require several simulation runs and need to be repeated for every operational regime of the simulated engine. A promising approach for the determination of a model's parameters is to inversely search for those effective parameters that yield the best fit between the measured and simulated results, using optimization methods. Optimization methods exclude time-consuming manual parameter determination, whilst also being more objective. For this kind of search we assume that a mathematical (thermodynamic or phenomenological) model would be able to precisely describe the physics of real conditions, and that the optimization method would be able to determine parameters values.

In this paper three different optimization methods for solving of inverse problem of parameter determination, were tested. Test was performed on one operating regime of ESC 13 mode test. Tested optimization methods were the quasi-Newton Broyden-Fletcher-Goldfarb-Shanno method (BFGS), the Gauss Newton Levenberg-Marquardt algorithm (L-M), and the genetic algorithm (GA). The objective function was expressed so, that minimize difference between experimentally determined in-cylinder pressure trace and in-cylinder pressure trace calculated by BOOST simulation program. From obtained results, the L-M method was selected as the most useful optimization method for determination of MCC combustion model parameters.

Inverse problem

The usage of optimization methods or methods of mathematical optimization is a well-known way for finding the best available value or optimum for some objective function, which can be either the maximum or minimum value of the given objective function. The primary task of optimization methods is to find optimal solutions for given function, where it is assumed that the parameters of the function or model are known, or at least can be determined in some way. In practice we can deal with cases, where the optimal solution is known or can be

determined experimentally, but what if we don't know the exact values of those model parameters that will give us this optimal result? In that case we can use optimization methods for determining model parameters based on known optimal solutions.

Model parameters are usually determined manually based on experimental results, which requires several simulation runs. Manually-based parameter determination can be very time-consuming and also inefficient when we need to determine several parameters. By using optimization methods, we can find model parameters that are also based on experimental results. This kind of parameter search (determination) is more systematical than a manual search, and without subjective influences.

Optimization methods can be divided into two sizeable groups, local and global optimization methods. The main difference between them is in the starting-point or initial-point of optimization. Local optimization methods start from a single initial-point within the parameter space. Starting in this way has a big influence on the probability of finding the global optimum and that is the main cause, while often local optimization methods cannot find the global minimum and thus terminate their searches prematurely. Contrary to the local optimization methods, global optimization methods start from several initial points within the parameter space. These methods enable a global search within the optimization space and reduce the probability of the optimization method getting stuck in the local optimum. Global search is the main advantages regarding global optimization methods such as Genetic algorithms, compared to the local-based optimization methods. However in order to find global optimum they need to evaluate more cases than local methods, which makes them much more time-consuming.

The local optimization methods used were the Broyden-Fletcher-Goldfarb-Shanno (BFGS) quasi Newton optimization method, and the Gauss-Newton algorithm named Levenberg-Marquardt (LM). The global optimization method used was the Genetic Algorithm for multi-objective optimization (GA).

Simulation model

AVL BOOST simulation program was developed for the numerical analyses of engine cycles, gas exchanges, exhaust gases after treatment and duct acoustics. A numerical (virtual) model of the whole engine was created so that comparisons between simulated and measured engine characteristics such as engine power and torque could be performed.

Many different combustion models are integrated within the BOOST program, and can be used for the calculations of engine performance. In the presented work a Chmela and Orthaber MCC combustion model was used for calculating the diesel engine's performance, and is presented in following section.

Combustion model

The amount of energy (heat) released during fuel combustion within the combustion chamber is the only source of energy input within internal combustion engines. Different authors have developed different combustion models for calculating heat-release within internal combustion engines. In our case Chmela and Orthaber's AVL MCC combustion model was used. The MCC combustion model divides the combustion into two stages, the first stage being the premixed or kinetic combustion dQ_{PMC}, which occurs after the ignition delay interval ends. The second part of the combustion is the mixing controlled or diffusion combustion dQ_{MCC}, which follows the premixed part of the combustion and begins when all the fuel/air mixture from the first part of the combustion has burned.

$$\frac{dQ_c}{d\alpha} = \frac{dQ_{total}}{d\alpha} = \frac{dQ_{MCC}}{d\alpha} + \frac{dQ_{PMC}}{d\alpha} \tag{1}$$

The amount of fuel vaporised and mixed with fresh air during the ignition delay interval is burned during the premixed part of combustion. The fuel/air mixture created during the ignition delay interval burns rapidly because of the large amount of excess air during this stage of combustion. The Vibe function was used for calculating the heat released from the premixed combustion. The classical Vibe function was used to describe the heat released $\frac{dQ_{PMC}}{Q_{PMC}}$ during the premixed part of combustion and is presented with equations (2) to (5):

$$\frac{\frac{dQ_{PMC}}{Q_{PMC}}}{d\alpha} = \frac{a}{\Delta\alpha_c}(m+1)y^m e^{-ay^{(m+1)}} \tag{2}$$

$$Q_{PMC} = m_{f,id}C_{PMC} \tag{3}$$

$$\Delta\alpha_c = \tau_{id}C_{PMC-Dur} \tag{4}$$

$$y = \frac{\alpha - \alpha_{id}}{\Delta\alpha_c} \tag{5}$$

The shape parameter m was set at 2 and the Vibe parameter a to 6.9 because the Vibe function was used for calculating the of heat released during the first part of combustion only. Duration of the ignition delay, τ_{id}, and the crank angle at which the ignition delay ends (start of combustion) α_{id} were calculated using an ignition-delay model developed by Andree and Pachernegg, equation (6), where I_{id} represents the ignition delay interval, T_{UB} the temperature of the unburned zone, and T_{ref} the reference temperature, which was set on 505K. $C_{PMC-Dur}$ in equation (3) present the premixed combustion duration factor.

$$\frac{dI_{id}}{d\alpha} = \frac{1}{C_{IDCF}}\frac{T_{UB} - T_{ref}}{Q_{ref}} \tag{6}$$

$$\tau_{id} = \alpha_{id} - \alpha_{SOI} \tag{7}$$

The ignition delay duration is calculated as the difference between the crank-angle at the start of injection α_{SOI} and the crank-angle at which the ignition delay ends and combustion occurs α_{id}.

In the mixing controlled part of the combustion burns fuel that was injected after the ignition has started. The model predicts that the amount of heat released in this stage of combustion dQ_{MCC} is a function of the fuel available for combustion $f_1(m_f, Q_{MCC})$ and the amount of local density regarding the turbulent kinetic energy present within cylinder $f_2(k, V_c)$ (8).

$$\frac{dQ_{MCC}}{d\alpha} = C_{comb}f_1(m_f, Q_{MCC})f_2(k, V_c) \tag{8}$$

The amount of fuel that is available for combustion is calculated as a function of the injected fuel m_f, and the amount of burned fuel $\frac{Q_{MCC}}{LCV}$.

$$f_1\big(m_f, Q_{MCC}\big) = \left(m_f - \frac{Q_{MCC}}{LCV}\right)\big(w_{O2,available}\big)^{C_{EGR}} \tag{9}$$

C_{EGR} is the parameter that allows user to regulate the amount of available oxygen's mass fraction, $w_{O2,available}$, if the engine has an exhaust gas recirculation valve (EGR).

The local density of turbulent kinetic energy k is a function of the mixing rate of constant C_{Rate} and cylinder volume V_c, and can be calculated using equations (11) and (12) when calculating kinetic energy E_{kin}.

$$f_2(k, V_c) = C_{Rate} \frac{\sqrt{k}}{\sqrt[3]{V_c}} \tag{10}$$

$$k = \frac{E_{kin}}{m_{f,inj}\big(1 + \lambda_{diff} m_{stoich}\big)} \tag{11}$$

$$\frac{dE_{kin}}{dt} = 0.5 C_{turb} \dot{m}_f \left(\frac{\dot{m}_f}{\rho_f \mu A}\right)^2 - C_{diss} E_{kin}^{1.5} \tag{12}$$

In equations (6), (8) and (12), we find those model parameters that are determined by the user, and as can be seen from the equations they have great influence on the results of numerical simulations. Their influence and control on the simulation results can be briefly described as:

- C_{IDCF} Ignition delay calibration factor (IDCF). It influences the ignition delay, higher values result in longer ignition delays and vice versa.
- C_{comb} Combustion parameter (CP). A higher value for this parameter assumes higher combustion speed. It has great influence on the shape of the rate of heat release curve.
- C_{turb} Turbulence parameter (TP). Using this parameter we can control the influence of kinetic energy on the simulation results.
- C_{diss} Dissipation parameter (DP). Using this parameter we can control the influence of dissipation on the simulation results.

The combustion model parameters are usually determined based on users' experience and knowledge of their influence on the combustion process. Their determination can also be presented as an inverse problem, and can be solved by use of optimization methods as method for solving of inverse problems.

Selection of optimization method
Combustion model determination was presented as inverse problem and was solved with use of optimization methods. The BFGS, L-M, and GA optimization methods were tested. The combustion model parameters were determined based on the experimental results of the measured in-cylinder pressure curves which were used as fitting parameters during the optimization process. In-cylinder pressure trace is one of more important parameters of an internal combustion engine. The form of the in-cylinder pressure trace has an influence on many engine characteristics, such as engine power, torque, rate of heat-release, soot, and other exhaust gas emission formations. Several phenomenological combustion models use in-cylinder pressure trace for calculating other phenomena that take place within an internal combustion engine.

The BOOST program was used as a program where numerical simulations were performed. The results from the numerical simulations were then sent to the IMPRESS Chart program where they were compared with the measured in-cylinder pressure curve (fitting parameter) for evaluating the objective function value (fitness). The results of the calculated objective function were then sent to the optimization method, which then used these results for calculating the function gradient and to evaluate new values for the combustion model parameters. The values for the new parameters were then sent to the simulation model in BOOST, where they were used as the new parameter values for the combustion model in new simulations. The optimization cycle was repeated until one of the termination criterion was reached (max number of iteration, minimal final termination accuracy or minimal finite difference between two steps).

The optimization process was defined as a single-objective optimization process because having only one fitting parameter, and can be written using equation (13), as:

$$\min F(x) \tag{13}$$

Where function F is presented as the continuous distribution function (14) for the BFGS and GA methods, and as a discrete function (15) for the L-M method.

$$F = \int \big(|f_{experiment} - f_{numerical}|\big)^2 \, d\alpha \tag{14}$$

$$F_{LM} = \frac{1}{2} \sum_{i=1}^{n} \big(x_{experiment_i} - x_{numerical_i}\big)^2; \quad n = 36 \tag{15}$$

A single-objective optimization problem requires only one objective function, which will be minimised. In our case, we decided to minimise the integral (14).

$$optif = \min(F) \tag{16}$$

The objective function $optif$ in (16) was set for the BFGS and GA optimization methods, whilst the objective function $optif_{LM}$ for L-M method was set as:

$$optif_{LM} = \min F_{LM} \tag{17}$$

Where $x_{experiment_i}$ and $x_{numerical_i}$ represent the experimental and numerical values for pressure at different angles α. When using the BFGS and GA optimization methods, the value of integral, equation (14), was minimized. The L-M optimization method requires discrete distribution of the objective function. The optimization method then tries to minimise the difference between the experimental results ($_{experiment}$) and simulation results ($_{numerical}$) at all 36 discrete points. The simulation model in BOOST, which was used for calculating the in-cylinder pressure curve, was set equally for all optimization methods.

Local optimization methods are very sensitive on the initial starting-point. A good starting-point will provide fast convergence to the optimum whilst a weak starting-point leads to slow convergence or even to premature termination of the optimization search. The ideal initial-point will be close to the minimums of each parameter. If the minimum is unknown, as in our case, the characteristic points of the parameter's interval are suitable starting points. The design of experiment was performed to find the search intervals of each parameter and to determine the initial points of each parameter, which were then set as centre values of the intervals for each parameter, Table 1

Table 1: Initial point and intervals of parameters

Parameter	Lower value	Upper value	Initial point
IDCF	0	2	1
CP	0	10	5
DP	0	10	5
TP	0	400	200

Results and discussion
Three different optimization methods with different searching techniques were tested in order to determine combustion model parameters using optimization methods. The test was performed on one operating regime of the ESC 13 mode. Table 2 presents some results for optimization using all three optimization methods, and experimental results of the selected operating regime.

Table 2: Inverse optimization results

Optimization method	Optimization steps	Torque [Nm]	Max. cylinder pressure [bar]	α of max cylinder pressure [°CA]
L-M	102	563	82.4	369
BFGS	134	566	84.4	369
GA	1800 (90 generations)	568	83.3	370
Experiment		540	82.7	369.7

As expected, the optimization method using the evolutionary searching technic (GA) was the most time-consuming method. It needed 90 generations to complete their search, which is equal to 1800 optimization cases. L-M and BFGS methods needed significantly less optimization steps than GA to provide almost the same results, as can be seen in Table 2 and in Figure 1.
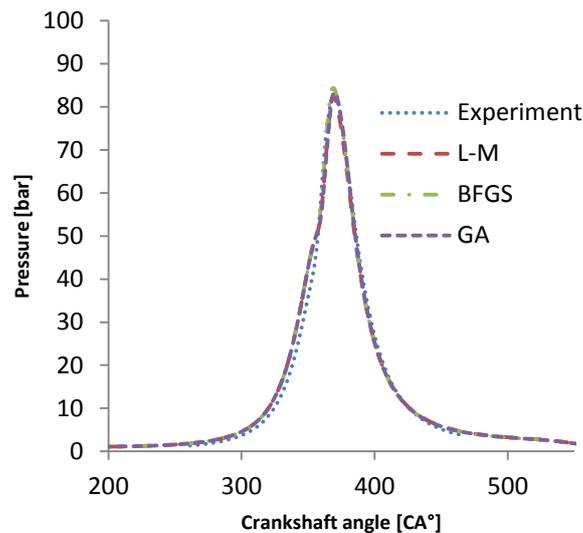

Figure 1: In-cylinder pressure obtained with different optimization methods

All the optimization methods were able to determine the combustion model parameters and their results agree well with the experimental results, presented in Table 1 and in Figure 1. L-M method was selected for determining the combustion model parameters for further work. The main advantages of L-M method are fast convergence (less computer cost), and good agreement with the experimental results.

Reference
[1] Kegl B. Influence of biodiesel on engine combustion and emission characteristics. *Appl. energy*. [Print ed.], May 2011, vol. 88, iss. 5, str. 1803-1812, doi: 10.1016/j.apenergy.2010.12.007.
[2] Hribernik A, Kegl, B. Influence of biodiesel fuel on the combustion and emission formation in a direct injection (DI) Diesel engine. *Energy fuels*. [Print ed.], 2007, vol. 21, iss. 3, str. 1760-1767.
[3] Lapuerta M, Armas O, Hernandez JJ, Tsolakis A. Potential for reducing emissions in a diesel engine by fuelling with conventional biodiesel and Fischer–Tropsch diesel.*Fuel*. [Printed ed.], 2010, vol. 89, page 3106-3113.
[4] Yamane K, Ueta A, Shimamoto Y. Influence of Physical and Chemical Properties of Biodiesel Fuel on injection, Combustion and Exhaust Emission Characteristics in a DI-CI Engine. *The Fifth International Symposium on Diagnostics and Modeling of Combustion in Internal COMBUSTION Engines (COMODIA)*. July 2001, Nagoya.
[5] Demirbas A. Progress and recent trends in biodiesel fuels. Energy conversion and Management. 2009, vol 50.
[6] Chmela F, Orthaber G. Rate of Heat Release Prediction for Direct Injection Diesel Engines Based on Purely Mixing Controlled Combustion. *SAE Technical Paper. 1999-01-0186*, 1999, doi:10.4271/1999-01-0186.
[7] Volmajer M, Kegl B. Diesel-spray analysis. *Journal of mechanical engineering.*, 2001, letn. 47, št. 10, str. 627-636.