Usage of optimization methods for determination of combustion model parameters

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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
The amount of fuel that is available for combustion is calculated as a function of the injected fuel amount of heat released in this stage of combustion which the ignition delay ends and combustion occurs. The ignition delay duration is calculated as the difference between the crank angle at which the ignition delay starts and combustion occurs, and the amount of burned fuel during the premixed part of combustion and is presented with equations (2) to (5):

\[
\frac{dQ_{\text{preM}}}{da} = \frac{a}{\Delta \alpha_c} (m + 1) y^m e^{-\alpha_c (m + 1)}
\]

\[
Q_{\text{preM}} = m_{\text{id}} e^{\Delta \alpha_c}
\]

\[
\Delta \alpha_c = \tau_{\text{id}} e^{\Delta \alpha_{\text{preM-dur}}}
\]

\[
y = \frac{a - a_{\text{id}}}{\Delta \alpha_c}
\]

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 heat released from the premixed combustion. The classical Vibe function was used to describe the heat released during the premixed part of combustion and is presented with equations (2) to (5):

\[
\frac{dQ_{\text{preM}}}{da} = \frac{a}{\Delta \alpha_c} (m + 1) y^m e^{-\alpha_c (m + 1)}
\]

\[
Q_{\text{preM}} = m_{\text{id}} e^{\Delta \alpha_c}
\]

\[
\Delta \alpha_c = \tau_{\text{id}} e^{\Delta \alpha_{\text{preM-dur}}}
\]

\[
y = \frac{a - a_{\text{id}}}{\Delta \alpha_c}
\]

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 heat released during the premixed part of combustion only. Duration of the ignition delay, \(\tau_{\text{id}}\), and the crank angle at which the ignition delay ends (start of combustion) \(a_{\text{id}}\) were calculated using an ignition-delay model developed by Andree and Pachernegg, equation (6), where \(\tau_{\text{id}}\) represents the ignition delay interval, \(T_{\text{ure}}\) the temperature of the unburned zone, and \(T_{\text{ref}}\) the reference temperature, which was set on 505K. \(e^{\Delta \alpha_{\text{preM-dur}}}\) in equation (3) present the premixed combustion duration factor.

\[
\frac{d\tau_{\text{id}}}{da} = \frac{1}{C_{\text{idCF}}} \frac{T_{\text{ure}} - T_{\text{ref}}}{Q_{\text{ref}}}
\]

\[
\tau_{\text{id}} = a_{\text{id}} - a_{\text{SOI}}
\]

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

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 \(dQ_{\text{MCC}}\) is a function of the fuel available for combustion \(f_i(m_f, Q_{\text{MCC}})\) and the amount of local density regarding the turbulent kinetic energy present within cylinder \(f_i(k, \gamma)\) (8).

\[
\frac{dQ_{\text{MCC}}}{da} = C_{\text{combF}} f_i(m_f, Q_{\text{MCC}}) f_i(k, \gamma)
\]

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 \(Q_{\text{MCC}}\).
\begin{equation}
  f_t(m_f, Q_{nec}) = \left( m_f - \frac{Q_{nec}}{LCV} \right) ^{c_{EGR}}
\end{equation}

\( c_{EGR} \) 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 \( E_{kin} \).

\begin{equation}
  f_k(k, V_c) = C_{rate} \left( \frac{k}{\sqrt{V_c}} \right)
\end{equation}

\begin{equation}
  k = \frac{E_{kin}}{m_{f,stoich} \left( 1 + \frac{\lambda_{dif} m_{stoich}}{\mu_f} \right)}
\end{equation}

\begin{equation}
  \frac{dE_{kin}}{dt} = 0.5 C_{turb} \rho_f \left( \frac{m_f}{\rho_f \mu_f} \right) - C_{diss} E_{kin}^{1.5}
\end{equation}

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:

\begin{equation}
  \text{min } F(x)
\end{equation}

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.

\begin{equation}
  F = \int \left( f_{\text{experiment}} - f_{\text{numerical}} \right)^2 \, dt
\end{equation}

\begin{equation}
  F_{LM} = \frac{1}{n} \sum_{i=1}^{n} \left( x_{\text{experiment}} - x_{\text{numerical}} \right)^2 ; \quad n = 36
\end{equation}

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

\begin{equation}
  \text{opt } f = \text{min } (F)
\end{equation}

The objective function \( \text{opt } f \) in (16) was set for the BFGS and GA optimization methods, whilst the objective function \( \text{opt } f_{LM} \) for L-M method was set as:

\begin{equation}
  \text{opt } f_{LM} = \text{min } F_{LM}
\end{equation}

Where \( x_{\text{experiment}} \) and \( x_{\text{numerical}} \) represent the experimental and numerical values for pressure at different angles \( \alpha \). 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 \( f_{\text{experiment}} \) and simulation results \( f_{\text{numerical}} \) 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>
<thead>
<tr>
<th>Parameter</th>
<th>Lower value</th>
<th>Upper value</th>
<th>Initial point</th>
</tr>
</thead>
<tbody>
<tr>
<td>IDCF</td>
<td>0</td>
<td>2</td>
<td>1</td>
</tr>
<tr>
<td>CP</td>
<td>0</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>DP</td>
<td>0</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>TP</td>
<td>0</td>
<td>400</td>
<td>200</td>
</tr>
</tbody>
</table>

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

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](image)

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**


