Application of Optimization Techniques to Determine Parameters of the Vibe Combustion Model

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The capability of the optimization algorithms employed for tuning parameters of the Vibe combustion model included in 1-D thermodynamic engine cycle simulation tool AVL BOOST is analyzed while simulating high pressure phase of the in-cylinder process. The objective of the analysis includes the ability check of the optimization methods to determine the parameters of the Vibe combustion model within the tolerance range needed to set up a high fidelity model and to reach accuracy threshold of the commonly applied analytic approach for determining combustion parameters. The employed method presents an influence of different merit functions and constraints on the accuracy of the results and proposes the methodology for their quality analysis. It can be concluded that the accuracy of the results calculated by combustion parameters determined by the optimization techniques reaches accuracy of the results calculated by a special analytically based software tool.

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0 INTRODUCTION

Software tools for thermodynamic modeling of internal combustion engines (ICEs) [1] to [4] have become indispensable for developing and optimizing the ICEs. Due to hardware performance constraints and due to computational time limitations, commercial simulation tools for modeling the complete internal combustion engine (ICE), including intake and exhaust manifolds, do not incorporate 3-D methods, or just take advantage of using coupling to the 3-D software to resolve phenomena in a specific selected component. Therefore, although the models are based on mechanistic models, they incorporate many tuning parameters needed to be adjusted to set up the high fidelity ICE simulation models. Tuning parameters have a clear physical interpretation and are, therefore, adjusted within a meaningful range characteristic for particular phenomena. Tuning parameters are employed due to the inability of the models to fully capture 3-D fluid flow and heat transfer phenomena, which are additionally coupled with mass transfer phenomena and chemical kinetics mechanisms during fuel injection, evaporation and combustion phase. Adjusting of a tuning parameter to meet the accuracy threshold required by the customers (agreement of measured and calculated engine performance should typically be in the range of 1

to 3%) is very time consuming and presents a considerable part of the work load of the whole project. Therefore, employment of optimization methods seems a promising approach for determining tuning parameters.

has already It been shown that optimization methods are suitable for determining optimized configurations of components, e.g. manifold geometry [5] and [6], shape of injection rate [7], exhaust gas recirculation (EGR) rates and multiple injections [8], injection timings [9], valve lift profiles and timings [6] and [10] to [13], as well as constants of heat transfer model [14]. These analyses either use a calibrated ICE simulation model as a starting point for evaluating optimized configuration [5], [6], [10], [12] and [13] or tune specific sub-model by optimization methods and compare simulation results to the experimental data [14].

The number of tuning factors (parameters) required to calibrate the simulation of the conventional turbocharged compression ignited ICE with variable turbine geometry (VTG) and EGR system, can vary in a range between 15 and 30. This might be inconvenient for an attempted employment of optimization methods to calibrate simulation model since the effectiveness of optimization techniques decreases with an increase the number of optimization factors. Therefore, it is proposed to divide the simulation model of ICE to feasible sub-systems and carry

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out the calibration process in two steps. The goal of the first step is to tune factors of sub-systems, while the goal of the second one is to adjust the reduced number of the most dominated parameters while optimizing the whole simulation model. Fig. 1 shows the proposed division of ICE simulation model into subsystems.

In the proposed study, the high pressure phase (HPP) of the in-cylinder process is analyzed (subsystem SS1_6 in Fig. 1) with the objective to analyze the ability of the optimization methods to determine the parameters of the combustion model within the tolerance range needed to set up a high fidelity model capable of reaching the above accuracy constraint. Therefore, engine performance data, in-cylinder combustion parameters, rate of heat release (ROHR) and pressure traces calculated by combustion parameters derived through optimization methods are compared to the measured and analytically derived data and to the data calculated by combustion parameters derived from analytically evaluated ROHR (commonly applied approach). Combustion parameters are determined through optimization methods by coupling of the optimization techniques with thermodynamic engine simulation model [1]. Analysis is performed with the design of experiments (DoEs) technique and NLPQL optimization method based on quadratic programming. Methods are included in software package [15]. Additionally, the influence of different merit functions on the determined tuning parameters is analyzed to reveal their substantial influence on the results.

In order to ensure high interpretative value of the analysis, a single Vibe combustion model was selected. It includes combustion duration (CD) and shape parameter m [16]. Moreover, the start of combustion (SOC) was also assigned as an optimization parameter, since it significantly influences engine performance.

1 HIGH PRESSURE PHASE AND SIMULATION MODEL

Cylinder process of ICE thermodynamic cycle includes an air plus, optionally, recirculated exhaust gas induction, compression, and combustion together with an expansion and exhaust phase. High pressure phase (HPP) comprises the cylinder process during the time period from the intake valve closing (IVC) to the exhaust valve opening (EVO).

Fig. 1 presents the proposed division of the ICE simulation model into subsystems marked with SS1 6, SS2 6, ..., SS6 6 for the case of the available measurement data labeled at positions $(0,1,\ldots,8)$. The division of the ICE model should depending on the available be driven measurement data. Quantities p_i , T_i denote static pressure and temperature at a certain position, whereas subscript *i* denotes *ref* refers ambient, 1 compressor inlet, 2 1 compressor outlet, 2 2 intercooler outlet, im intake manifold, 3 turbine inlet and 4 conditions at turbine outlet. \dot{m}_{air} and \dot{m}_{fuel} represent air and fuel mass flow rate, respectively, P_{en} brake power and n rotational speed of ICE. SS1 6 covers cylinder with HPP, SS2 6 inlet orifice - compressor inlet, SS3 6 compressor outlet - intake manifold inlet, SS4 6 turbine outlet - exhaust orifice, SS5 6 turbocharger with compressor/turbine inlet and outlet, SS6 6 intake manifold inlet, engine block with cylinders, exhaust manifold outlet (up to turbine inlet).

The required condition enabling evaluation of the HPP in the cylinder e.g. with [1] or [17] is initial thermodynamic state (ITDNS) in the cylinder at the time of IVC. During HPP incylinder variables are not influenced by other engine components, since the intake and exhaust valves are closed, and thus only ITDNS is influenced by other engine components (e.g. intake/exhaust system during gas exchange process). ITDNS is determined either by the cylinder pressure at IVC (p_{cyl} _{IVC}), \dot{m}_{air} , \dot{m}_{fuel} and residual gas concentration (RGC), or by the temperature, pressure and gas compositions at IVC. Gas compositions are defined by air to fuel ratio, fuel vapour and combustion products concentration. The application of the measured data for p_{cvl} IVC, \dot{m}_{air} , \dot{m}_{fuel} and estimated RGC for HPP analysis, excludes the impact of the other engine components. RGC cannot be measured. It is, therefore, determined either by specialized software tools, e.g. [1] and [18] where complete ICE cycle has to be simulated, or based on the user experience. For presented work RGC values have been determined based on the user experience.



Fig. 1. Conceptual division of ICE into subsystems

The objective of the HPP thermodynamic analysis is to determine appropriate ROHR resulted from in-cylinder combustion process based on known (measured) cylinder pressure trace and ITDNS. The determination of the ROHR from the measured data is commonly performed by the analytical method via specialized software tools, e.g. [17] and [18]. This gives ROHR as a function of the CA rotation (table). Besides, [17] and [18] also evaluate SOC and Vibe combustion model parameters (CD, m) from ROHR by analytical approach. Optionally also, a direct approach to tune parameters of a certain combustion model included in [1] might be applied. Thereby, sufficiently good agreement in simulated and measured pressure represents the target for parameters tuning of certain combustion model. Tuning of the combustion model parameters through the direct approach can be realized by performing simulations with an activated check box start high pressure (SHP) within the cylinder element of the simulation model presented in Fig. 2 either with an application of trial-and-error method or by optimization techniques. The latter has been carried out in the presented work.

The input factors of the selected combustion model being the subject of optimization tuning have to be assigned as variables (parameters). [1] includes several physical models for ROHR prediction whose number of tuning parameters depends on the complexity of certain model. A single Vibe model was applied in the analysis, since it enables a comparison between parameters evaluated with [17] and the same set of parameters determined directly with an optimization techniques.



Fig. 2. Simulation model created with [1] for combustion model parameters tuning

A simulation model consists of a cylinder element (C1), attached pipes 1, 2 that model intake and exhaust port, and internal boundaries (IB1, IB2) that involve static boundary conditions (e.g. pressure, temperature) at a certain position in the intake and exhaust port. ITDNS for HPP analysis is determined in SHP input dialog. The required input data for IB1, IB2 conditions and for pipes 1 and 2

attached to the C1 do not influence the simulation results, but they have to be specified due the layout structure of [1].

The measured data of MAN turbocharged compression ignited (TCI) diesel engine were used for the presented work. Basic engine geometry and valve timings are listed in Table 1.

Table 1. Engine geometry and valve timings of6.87L MAN TCI diesel engine

Bore [m]	0.108					
Stroke [m]	0.125					
Connection rod length [m]	0.1825					
Compression ratio [-]	18					
Piston pin offset [m]	0.0005					
IVO [CA]	17 BTDC = 343					
IVC [CA]	33 ABDC = 573					
EVO [CA]	57 BBDC = 123					
EVC [CA]	25 ATDC = 385					
Number of valves/cylinder	2					
Number of cylinders	6					
Cylinder displacement [1]	1.145					
Engine displacement [1]	6.87					

Valve timings are specified according to firing top dead center (FTDC) determined in [1] with 0 CA.

2 CYLINDER BALANCE EQUATIONS

In a 0-D single zone model, balance equations of mass, energy and species concentrations form a sufficient set of dependent variables, and time or equivalently crank angle rotation represents the independent variable. Fig. 3 shows a physical model and state variables of the cylinder and intake/exhaust ports.



Fig. 3. Schematic of the considered four-stroke cylinder connected to the intake and exhaust

manifold including state variables and fluxes

The framework of balance equations is laid out in a general way enabling a consideration of an arbitrary number of species

$$\boldsymbol{W} = \begin{bmatrix} w_1 \dots w_m \end{bmatrix}^T . \tag{1}$$

In the presented analysis species vector W, represents burned fuel (FB), combustion products (CP) and fuel vapor (FV).

$$\boldsymbol{W} = \left[w_{FB}, w_{CP}, w_{FV} \right]^T \tag{2}$$

whereas species concentration of air is derived by:

$$w_{air} = 1 - w_{CP} - w_{FV}$$
. (3)

In deriving governing equations the dependency of internal energy (u)

$$u = u(T, p, w_1 \dots w_{m+1})$$
(4)

and specific gas constant (R)

$$R = R(T, p, w_1 \dots w_{m+1})$$
(5)

on temperature (*T*), pressure (*p*), and species concentrations (w_{FB} , w_{CP} , w_{FV} , w_{air}) are considered.

A revised ideal gas equation [19]:

$$pV = m\frac{Z\Re}{M}T = mRT \tag{6}$$

adequately captures deviations of the real gas from the ideal one in the range of temperatures and pressures characteristic for the in-cylinder processes of ICEs; herein V is volume, m is mass, Z is compressibility factor, \Re is universal gas constant and M molar mass.

The mass balance equation is:

$$\frac{\mathrm{d}m}{\mathrm{d}\varphi} = \sum_{j}^{n_{values}} \frac{\mathrm{d}m_j}{\mathrm{d}\varphi} + \frac{\mathrm{d}m_{inj}}{\mathrm{d}\varphi} + \frac{\mathrm{d}m_{bb}}{\mathrm{d}\varphi}$$
(7)

where φ is the independent variable representing CA rotation, and indexes *inj* injection and *bb* blow-by. The change of mass depends on the fluxes through the attached valves and the amount of the injected fuel.

The rate of change of species conservation comprises species concentration variation due to mass transfer and species concentration variation due to:

$$\frac{\mathrm{d}w_{k}}{\mathrm{d}\varphi} = \frac{\sum_{j}^{n_{\mathrm{values}}} \left(w_{k,d} - w_{k,cyl}\right) \frac{\mathrm{d}m_{j}}{\mathrm{d}\varphi}}{m} + \frac{\mathrm{d}w_{k,C}}{\mathrm{d}\varphi}$$
(8)

where index d denotes

$$d = \begin{cases} cylinder & \text{for } dm \le 0\\ plenum & \text{for } dm > 0 \end{cases}.$$
(9)

The first law of thermodynamics for an open system equals

$$\mathrm{d}U = \mathrm{d}Q - p\mathrm{d}V + \mathrm{d}H \tag{10}$$

where

$$\mathrm{d}Q = \mathrm{d}Q_C + \mathrm{d}Q_{HT} \tag{11}$$

$$dH = \sum_{j}^{n_{valves}} h_d dm_j + h_{bb} dm_{bb}$$
(12)

and index d is defined by eq. (9).

Term dQ_C in Eq. (11) models rate of heat release (ROHR) while dQ_{HT} in Eq. (11) models heat flux from the gas within the combustion chamber to the surrounding walls. ROHR according to Vibe model [16] is determined by the following equation

$$\frac{\mathrm{d}Q_{\mathrm{C}}}{\mathrm{d}\varphi} = Q_{F} \frac{\mathrm{d}x_{\mathrm{b}}}{\mathrm{d}\varphi} = LHVm_{inj} \frac{a}{\Delta\varphi} (m+1) \left(\frac{\varphi - \varphi_{0}}{\Delta\varphi}\right)^{m} e^{-a \left(\frac{\varphi - \varphi_{0}}{\Delta\varphi}\right)^{(m+1)}}$$
(13)

where $Q_{\rm F} = m_{\rm inj}LHV$ denotes fuel energy, $m_{\rm inj}$ mass of the fuel injected into the cylinder, *LHV* lower heating value of the fuel, *a* completeness of combustion [16], $\Delta \varphi$ combustion duration [16], φ_0 start of combustion and *m* shape factor [16].

A general equation for heat transfer (to the walls) evaluation considered in [1] has a form

$$\frac{\mathrm{d}Q_{HT}}{\mathrm{d}\varphi} = A_i \alpha_w(\varphi) HTCF(T(\varphi) - T_{w,i})$$
(14)

where A_i represents the surface area of the surrounding walls, e.g. (cylinder head, piston liner), a_w heat transfer coefficient [20], *HTCF* heat transfer multiplier, $T_{w,i}$ wall temperature of the surface A_i . Index *i* denotes cylinder head, piston or liner.

The thermodynamic engine cycle simulation model [1] calculates in-cylinder temperature and pressure due to mass and enthalpy flows, combustion and piston kinematics. Therefore, Eq. (10) is algebraically reformulated to be explicit in temperature leading to (derivation was done in analogy to [21] where additionally a more general dependency of the internal energy (Eq. (4)) and the gas constant (Eq. (5)) on species concentration is taken into account)

$$\frac{\mathrm{d}T}{\mathrm{d}\varphi} = \frac{B}{m} \left[\frac{\mathrm{d}Q}{\mathrm{d}\varphi} + \frac{\mathrm{d}H}{\mathrm{d}\varphi} + (Km-1) \right]$$
$$p \frac{\mathrm{d}V}{\mathrm{d}\varphi} - (u + KTRm) \frac{\mathrm{d}m}{\mathrm{d}\varphi}$$
$$- m \left(KmT \frac{\partial R}{\partial w_k} + \frac{\partial u}{\partial w_k} \right) \frac{\mathrm{d}w_k}{\mathrm{d}\varphi} \right]$$
(15)

where

$$K = \frac{\partial u}{\partial p} \frac{1}{V\left(1 - \frac{p}{R} \frac{\partial R}{\partial p}\right)}$$
(16)

and

$$B = \frac{1}{KmR\left(1 + \frac{T}{R}\frac{\partial R}{\partial T}\right) + \frac{\partial u}{\partial T}}$$
(17)

The direct approach of combustion model parameters tuning (SOC, CD, m) via the optimization technique is based on the coupling of the optimization techniques with thermodynamic engine simulation model [1] based on the Eq. (15).

Combustion analysis is based on the inverse procedure where ROHR is calculated from measured pressure trace, piston kinematics, heat transfer, and ITDNS data. Therefore, Eq. (4) is algebraically reformulated to

$$\frac{dQ}{d\varphi} + \frac{dH}{d\varphi} - \left(1 + \frac{1}{RA}\frac{\partial u}{\partial T}\right)p\frac{dV}{d\varphi} - \left(u - \frac{T}{A}\frac{\partial u}{\partial T}\right)dm - \frac{\partial u}{\partial w_k} - T\frac{\frac{\partial u}{\partial T}\frac{\partial R}{\partial w_k}}{RA}dw_k - m\left(\frac{\partial u}{\partial p} + \frac{TC}{pA}\frac{\partial u}{\partial T}\right)dp = 0$$
(18)

where:

$$A = 1 + \frac{T}{R} \frac{\partial R}{\partial T}$$
(19)

and

$$C = 1 - \frac{p}{R} \frac{\partial R}{\partial p} \,. \tag{20}$$

Analytic determination of the ROHR from the measured data is performed via specialized software tool [17] based on Eq. (18).

3 COMBUSTION MODEL PARAMETERS TUNING WITH OPTIMIZATION METHODS

The proposed study was investigated with the combination of DoE and NLPOL optimization included method in the optimization software package [15]. DoE method was used to determine feasible design space of tuning factors (parameters) and to determine a good starting point for a further process optimization employing NLPOL algorithm. NLPOL [15] and [22] is gradient based local optimization method, which requires a good starting point close to the global minimum or the merit function must be convex featuring only one local minimum. The purpose of DoEs is to gain a maximum amount of information about the simulation model response, while minimizing the number of simulations. Full factorial design (FFD) [15] was implemented for factors screening. Factors by which minimum merit function was attained have been used as a starting point for optimization process. Based on former analyses it was decided to perform optimization with NLPQL instead of e.g. genetic algorithm, since combining DoEs and NLPQL methods requires significantly less iterations (5 to 10 times) to attain the similar accuracy of the results.

The following steps were performed in tuning the Vibe combustion model parameters using DoEs and NLPQL optimization algorithms:

 Preprocessing measured cylinder pressure trace and analytical evaluation the ROHR.
 [17] includes options to filter the measured cylinder pressure trace in order to compensate for noise, errors or inaccuracies. Besides top dead center (TDC) and pressure offset error can be detected. A preprocessed measured cylinder pressure trace was later used for an analytical evaluation of the ROHR based on Eq. (18) considering the measured ITDNS as well for the optimization process. Besides, the calculated Vibe parameters (*m*, *CD*), SOC, and CA rotations at 5% ($\varphi_{5\%MFB}$) and 90% ($\varphi_{90\%MFB}$ burnt mass fractions were extracted from [17].

- 2. Geometric parameterization. The desired tuning factors of Vibe combustion model (m, CD) and SOC used in the simulation model presented in Fig. 3 were assigned to the variables enabling their variation during optimization.
- 3. The simulation of the response and the definition of the optimization objectives. With the initial set of tuning factors (m, CD, SOC) one simulation was performed by [1] and afterwards merit and constraints functions were determined by [23]. Single and multi-objective optimization problems were dealt with equality constraints. Besides, selected merit functions were analyzed also as an unconstrained optimization problem with the aim to reveal influence of the constraints. The optimization problem is expressed with the following equations:

 $\min F(x)$

Subject to:

$$h_{i}(x) = 0 \quad i = 1 \dots 4$$

$$x = [x_{1}, x_{2}, x_{3}] = [m, CD, SOC]$$

$$x_{k}^{l} \le x_{k} \le x_{k}^{u} \quad k = 1 \dots 3$$
(21)

whereas F(x) represents single or multiobjective merit function, $h_i(x)$ equality constraint and x vector of tuning factors.

Four different single $(F_{1,2,4,5})$ and two multi-objectives merit $(F_{3,5})$ functions have been investigated:

$$F_{1}(\mathbf{x}) = \frac{1}{C_{DUR}} \int_{\varphi_{IVC}}^{\varphi_{EVO}} (p_{cyl_{-}s}(\mathbf{x}, \varphi) - p_{cyl_{-}m}(\varphi))^{2} d\varphi$$
(22)

$$F_{2}(\mathbf{x}) = \frac{1}{C_{DUR}} \int_{\varphi_{IVC}}^{\varphi_{EVO}} \left(\frac{\mathrm{d}Q_{F_{s}}}{\mathrm{d}\varphi} (\mathbf{x}, \varphi) - \frac{\mathrm{d}Q_{F_{s}}}{\mathrm{d}\varphi} (\varphi) \right)^{2} \mathrm{d}\varphi$$

$$(23)$$

$$F_3(\mathbf{x}) = F_1(\mathbf{x}) + F_2(\mathbf{x}) \tag{24}$$

$$F_{4}(\mathbf{x}) = \frac{1}{C_{DUR}} \int_{\varphi_{5\%MFB}}^{\varphi_{90\%MFB}} p_{cyl_{-}s}(\mathbf{x}, \varphi)$$
$$- p_{cyl_{-}m}(\varphi)^{2} d\varphi$$
(25)

$$F_{5}(\mathbf{x}) = \frac{1}{C_{DUR}} \int_{\varphi_{5\%_{MFB}}}^{\varphi_{90\%_{MFB}}} \left(\frac{\mathrm{d}Q_{F_{s}}}{\mathrm{d}\varphi}(\mathbf{x}, \varphi) - \frac{\mathrm{d}Q_{F_{s}}}{\mathrm{d}\varphi}(\varphi) \right)^{2} \mathrm{d}\varphi$$

$$(26)$$

$$F_6(\mathbf{x}) = F_4(\mathbf{x}) + F_5(\mathbf{x}) \tag{27}$$

whereas index <u>s</u> denotes parameters evaluated by [1], <u>a</u> denotes analytically determined parameters [17], and <u>m</u> denotes measured quantity. C_{DUR} represents cycle duration of 4stroke ICE in CA rotation (720 CA), φ_{IVC} , φ_{EVO} timings of IVC, EVO, p_{cyl} cylinder pressure trace and $dQ_{\text{F}}/d\varphi$ ROHR.

Merit functions were constructed in a way that pressure deviation, ROHR deviation or both were integrated during the complete HPP or only during $\varphi_{5\%MFB}$ and $\varphi_{90\%MFB}$. Thereby it was analyzed if it is more appropriate to evaluate merit functions during complete HPP or only during the period of intensive combustion.

Equality constraints have been derived based on difference between measured and simulated quantities as

$$h_{1}(\mathbf{x}) = \frac{1}{V_{sw}} \int_{\varphi_{IVC}}^{0} \left(p_{cyl_{m}} - p_{cyl_{s}} \right) \mathrm{d}V$$
(28)

$$h_2(\mathbf{x}) = \frac{1}{V_{sw}} \int_0^{\varphi_{EVO}} \left(p_{cyl_m} - p_{cyl_s} \right) \mathrm{d}V$$
(29)

$$h_{3}(\mathbf{x}) = \max\left(p_{cyl_{m}}\right) - \max\left(p_{cyl_{s}}\right)$$
(30)

$$h_4(\mathbf{x}) = \varphi\left(\max\left(p_{cyl_m}\right)\right) - \varphi\left(\max\left(p_{cyl_s}\right)\right) \quad (31)$$

where V_{sw} represents cylinder displacement and $\max(p_{cyl})$ represents peak-firing-pressure (PFP).

The definition and execution of DoEs and NLPOL optimization algorithms using [15] in co-simulation with [1]. The definition includes a specification of the lower and upper bounds of design variables (tuning factors), target of the merit functions (Minimum or Maximum), definition the type (equality, nonequality) and the input values of constraints, optimization method selection. During the execution [15] defines values of the tuning factors according to the plan generated by the employed DoE or optimization algorithm. The values of the tuning factors are passed to the simulation model [1], which returns the quantities being the subject of the optimization process. The process is running in the loop until convergence criterion is reached. In the case of DoE the number of iterations is fixed and depends on the design plan (e.g. FFD).

4 RESULTS AND ANALYSIS

In the proposed study two different engine operating speeds (1600 and 2400 rpm) at full load have been analyzed applying 6 merit functions defined by Eqs. (22) to (27). For each Vibe combustion model engine speed. parameters of the best design were extracted from [15] and passed to the Case Explorer of [1] for all merit functions. Cycle simulation results [1] evaluated by Vibe parameters obtained through optimization techniques and by Vibe parameters determined by an analytic approach [17] were compared to the measured cylinder pressure trace and analytically calculated ROHR using a post-processing tool [23]. Furthermore, quality analysis (QA) of the results was performed with the aim to reveal the merit function featuring the best match to the measured cylinder pressure trace. Thereby deviations of indicated mean effective pressure of the HPP ($\Delta IMEP_{SHP}$), peak firing pressure $(\Delta p \text{ max})$, SOC (ΔSOC) , CA rotation of PFP $(\Delta \varphi_{p \text{ max}})$ and over all deviation (Δall) were analyzed, where:

$$\Delta IMEP_{SHP} = (IMEP_{SHP}_{s} - IMEP_{SHP}_{m})/IMEP_{SHP}_{m}$$
(32)

$$\Delta p \max = \left(\max \left(p_{cyl_s} \right) - \max \left(p_{cyl_m} \right) \right) / \max \left(p_{cyl_m} \right)$$
(33)

$$\Delta SOC = \left(\frac{SOC_{_s} - SOC_{_a}}{SOC_{_a}}\right)$$
(34)

$$\Delta \varphi_{p \max} = \frac{\left(\varphi_{p \max_s} - \varphi_{p \max_m}\right)}{\varphi_{p \max_m}} \tag{35}$$

$$\Delta all = |\Delta IMEP_{SHP}| + |\Delta p \max| + |\Delta SOC| + |\Delta \varphi_{p \max}|$$
(36)

and

$$IMEP_{SHP_{i}} = \frac{1}{V_{SW}} \int_{\varphi_{IVC}}^{\varphi_{EVO}} p_{cyl_{i}} dV$$
(37)

index *i* in Eq. (37) denotes either measured or simulated cylinder pressure trace and φ_{pmax} in Eqs. (35) and (36) CA rotation of PFP. QA of the results was performed by using scripts programmed in [24]. Δall was defined as a sum of all quality parameters (Eqs. (32) to (35)) to give a basic lumped information on the quality of particular method, since $\Delta IMEP_{SHP}$ directly influences engine performance and other parameters directly or indirectly influence engine emissions. The measured values given in the row 1-M of Tables 2 and 3 have been used as a reference for QA.

Fig. 4 shows cylinder pressure traces (a) and (b) and ROHR (c) for the engine speed 1600 rpm, where 1-M denotes measured pressure trace, 2-Va denotes pressure trace calculated by analytically determined parameters applying [17], and 3-VF1, 4-VF2, ..., 8-VF6 denote pressure trace calculated by combustion parameters obtained through optimization techniques (3-VF1 corresponds to the parameters determined by merit function F_1 (Eq. (22)), 4-VF2 merit function F_2 (Eq. (23)), ... and 8-VF6 merit function F_6 (Eq. (27))).

It is discernable from Fig. 4 a that agreement of all pressure traces is well until SOC and late in the expansion phase. Therefore, a detailed analysis is focused on the early combustion phase shown in Fig. 4 b and on the quality parameters. Fig. 4 b shows that different methods to determine combustion parameters significantly influence agreement in pressure traces, which results from the differences in the ROHR (Fig. 4 c). Due to the fact that Vibe combustion model includes only two parameters and SOC represents an additional tuning parameter, it is expected that ROHR curves calculated by the Vibe model could not fully coincide with the analytically derived ROHR as shown in Fig. 4 c. By analyzing curves 2-Va it can be concluded that the analytical method determines SOC very accurately (Fig. 4 c and Table 2), whereas it significantly underpredicts the maximum ROHR resulting in large deviation of the PFP (Fig. 4 c and Table 2).



Fig. 4. Measured and simulated cylinder pressure traces and ROHR at 1600 rpm

By analyzing the curves 3-VF1...8-VF6 it can be concluded that merit functions considering complete HPP generally better comply with the qualitative and quantitative accuracy criteria. It is discernable from Fig. 4 and Table 2 that VF2, VF4 and VF6 predict retarded SOC resulting in the initial pressure

drop after TDC. VF2 aims to fit best the analytically derived ROHR without any constraint on the SOC, whereas VF4 and VF6 consider only data after $\varphi_{5\%MFB}$. It is further discernable that VF1 and VF3 that totally or partially aim to fit pressure trace in HPP follow pressure trace with the smallest deviations. It is quite obvious that VF5 features the largest discrepancies, since it only fits ROHR between 5 and 90% MFB and, therefore, predicts too large ROHR values until 5% MFB resulting in too large pressure gradient. By analyzing Table 2 it can be concluded that for 1600 rpm, analytic method features the smallest discrepancy in IME_{SHP} , whereas it is possible to better resolve pressure and thus also temperature in the vicinity of their maximum values by the combustion parameters determined through optimization methods. The latter is of a particular importance when modeling engine emissions.

Fig. 5 shows cylinder pressure traces (a) and (b) and ROHR (c) for the engine speed 2400 rpm. It can be seen from Fig. 5 a that pressure is falling during the complete ROHR phase and thus, maximum cylinder pressure coincides with the compression pressure. Therefore, the results of all the methods give identical results of $\Delta \varphi_{pmax}$ and very similar results of $\Delta pmax$ (Table 3). Furthermore, it can be seen that the analytical method and both optimization methods that feature the best Δall values give very similar ROHR curves. All these curves coincide well with the analytically derived ROHR curve, particularly during early combustion phases. It can, therefore, be observed that values of $\Delta IMEP_{SHP}$ are very small for 2400 rpm case. By analyzing Table 3 it can be concluded that for this engine speed selected optimization techniques outperform analytic method for determining combustion parameters for all quality parameters.

An additional analysis was performed to analyze the influence of applying optimization constrains (Eqs. (28) to (31)) on the engine parameters. Thereby, the unconstrained optimization problem was executed for merit functions featuring the best optimization objectives for constrained optimization problem. By analyzing Tables 2 to 4 it can be concluded that, except for F1 at 1600 rpm, results obtained by the constrained optimization problem feature slightly lower overall deviation (Δall). However, a more important conclusion can be drawn form the comparison of the SOC values. It can be concluded that unconstrained optimization problem consistently evaluates retarded SOC values. This might have negative influences on the exhaust emission models, since retarded SOC is compensated by the larger initial ROHR gradient. Based on these facts a constrained optimization problem is preferred to apply.



Fig. 5.: Measured and simulated cylinder pressure traces and ROHR at 2400 rpm

optimization	problem								
Engine Speed	1600 [rpm]								
Label	SOC	IMEP _{SHP}	pmax	φ_{pmax}	$\Delta IMEP_{SHP}$	$\Delta pmax$	$\Delta \varphi_{pmax}$	ΔSOC	Δall
Laber	[CA]	[bar]	[bar]	[CA]	[%]	[%]	[‰]	[‰]	[%]
1-M	718.00	15.90	124.34	734.00	/	/	/	/	/
2-Va	718.46	15.85	118.22	731.00	-0.32	-4.93	-4.09	0.64	5.71
3-VF1	718.56	16.19	125.05	732.00	1.85	0.56	-2.72	0.78	2.77
4-VF2	722.18	16.16	124.47	733.00	1.67	0.10	-1.36	5.81	2.49
5-VF3	719.12	16.16	124.61	732.00	1.68	0.21	-2.72	1.55	2.32
6-VF4	722.86	16.07	125.77	733.00	1.11	1.15	-1.36	6.76	3.07
7-VF5	718.08	16.32	131.98	732.00	2.66	6.14	-2.72	0.11	9.09
8-VF6	723.00	16.11	126.15	733.00	1.36	1.45	-1.36	6.96	3.65

 Table 2. Reference values and results of the quality analysis at 1600 rpm by dealing with constrained optimization problem

Table 3. *Reference values and results of the quality analysis at 2400 rpm by dealing with constrained optimization problem*

Engine Speed	2400 [rpm]								
Label	SOC [CA]	<i>IMEP_{SHP}</i> [bar]	<i>pmax</i> [bar]	φ_{pmax} [CA]	$\Delta IMEP_{SHP}$ [%]	$\Delta pmax$ [%]	$\Delta \varphi_{pmax}$ [%0]	ΔSOC [‰]	Δall [%]
1-M	716.00	14.15	127.69	720.00	/	/	/	/	/
2-Va	720.45	14.09	127.92	720.00	-0.44	0.18	0.00	6.22	1.25
3-VF1	722.24	14.13	127.92	720.00	-0.18	0.18	0.00	8.71	1.24
4-VF2	719.74	14.16	127.93	720.00	0.04	0.19	0.00	5.22	0.75
5-VF3	719.78	14.10	127.93	720.00	-0.35	0.18	0.00	5.27	1.06
6-VF4	723.65	14.10	127.92	720.00	-0.39	0.18	0.00	10.68	1.64
7-VF5	719.63	14.32	127.93	720.00	1.22	0.19	0.00	5.07	1.92
8-VF6	719.55	14.22	127.94	720.00	0.50	0.19	0.00	4.96	1.19

Table 4. SOC values and results of the quality analysis at 1600 and 2400 rpm by dealing with unconstrained optimization problem

Engine Speed		1600 [rpm]		2400 [rpm]			
Label	3-VF1	4-VF2	5-VF3	3-VF1	4-VF2	5-VF3	
SOC [CA]	720.84	720.73	721.21	722.00	722.37	722.47	
$\Delta IMEP_{SHP}$ [%]	1.21	1.55	1.39	-0.29	0.29	0.03	
$\Delta pmax$ [%]	-0.15	1.03	0.92	0.18	0.18	0.18	
$\Delta \varphi_{pmax}$ [%o]	-2.72	-2.72	-2.72	0.00	5.27	1.06	
ΔSOC [‰]	3.95	3.80	4.47	8.38	8.90	9.03	
Δall [%]	2.03	3.23	3.03	1.31	1.36	1.11	

5 CONCLUSIONS

In the proposed study the high pressure phase of the in-cylinder process is analyzed with the objective to analyze the ability of the optimization methods to determine the parameters of the Vibe combustion model within the tolerance range needed to set up a high fidelity model. Qualitative and quantitative comparisons of the results showed three major points. First, optimization techniques are applicable for combustion parameter tuning if the adequate merit function is applied. Second, optimization techniques are capable to determine combustion parameters in the tolerance range required to model thermodynamic in-cylinder parameters with high fidelity. Third, the accuracy of the results calculated by combustion parameters determined by optimization techniques reaches the accuracy of the results calculated by combustion parameters determined by the analytic method through a special software tool [17]. It can be concluded that merit functions integrated over the complete HPP generally feature higher accuracy results. It can also be concluded that an application of optimization constraints generally increases the accuracy of the results. It was shown that optimization techniques are capable to determine combustion parameters for measured pressure traces featuring different characteristics (e.g. pressure rise after SOC, φ_{pmax}).

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