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NON-LINEAR PARAMETER ESTIMATION IN DIESEL ENGINE SIMULATION

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Abstract. *This paper aims to calculate parameters of a CFR diesel engine cetane testing backed by the standard ASTM D613. This process is carried through the means of an inverse analysis. The initial conditions for pressure and temperature are assumed unknown. As a means to quantify the sought parameters, pressure measurements are assumed to be available during the compression stroke of the diesel cycle. In order to achieve the proposed goal, simulations based on physical models are performed to quantify numerically the pressure curves to be compared and fitted to the experimental data. Relevant parameters such as cylinder pressure and temperature are taken into account. Some of these parameters may also not be directly measurable, due to hazardous conditions to which the probes would be subjected. Thus, the inverse analysis play an important role in such scenario. A parameter estimation is performed using the Levenverg-Marquardt algorithm and the estimates present good agreement with reference values. Also, the solution of the inverse problem is achieved with relatively low computational cost. Such methods can provide tools for researchers and engineers to design more efficient and environmentally friendly engines.*

Keywords: Diesel Engine, Parameter Estimation, Numerical Analysis

1. INTRODUCTION

Diesel engines play an important role in society, then researchers and engineers are interested to perform its modelling. According to Merker *et al.* (2005), there are several approaches for diesel combustion modelling, such as zero-dimensional heat release function, stationary gas jet, packet models and time scale models. In fact, this work uses such zero-dimensional models, due to its short calculation time and simple application when compared with other approaches. Thus rendering them is very useful for the intents and purposes given herein.

From the thermodynamics, the internal energy of the gas within the engine cylinder can be modelled from a number of parameters, allowing it to be evaluated theoretically. Moreover, the gas composition is usually assumed homogenous.

Data acquisition can have setbacks during experimental procedures. For example, acquiring directly temperature data from combustion chamber would expose the probe to high temperatures as as fast and intense temperature gradients, which might present a severely hazardous situations. Therefore, it needs to resort to indirect measurement techniques in such scenarios using information somewhat related to the observed phenomena. Research dedicated to solving those problems is associated with the area known as inverse problems. In terms of engine simulation, relevant studies have been performed by Rida *et al.* (2016), Payri *et al.* (2011) and others.

Quantifying the chamber pressure is crucial for diesel engines due its combustion mechanism that uses high compression fuel. However some setbacks regarding data acquisition may require an inverse analysis in order evaluate missing information. The research presented in this paper is based on thermodynamical and mechanical models described by Heywood (1988) and Merker *et al.* (2005).

The goal of this paper is to use pressure measurements, obtained inside the combustion chamber during the compression stroke to estimate initial conditions of temperature and pressure, which have a direct influence to those measurements.

2. PHYSICAL MODEL

The diesel engine geometry is shown in Figure 1, where its cylinder moves from its bottom dead centre (BDC) to its top dead centre (TBC). Then, the engine's geometrical parameters being obtained from ASTM (2018). Furthermore, the geometry consists of a crank-slider mechanism with a crank radius r of 57.15 mm and a connecting rod length l of 254 mm, which provides the work done by the piston due the chamber pressure. The bore B is assumed to be of 82.55 mm, the stroke S to be of 114.3 mm. It is considered an engine with compression ratio r_c ranging from 8 to 36. Also, its swept volume V_{swept} has 611.73 cc.
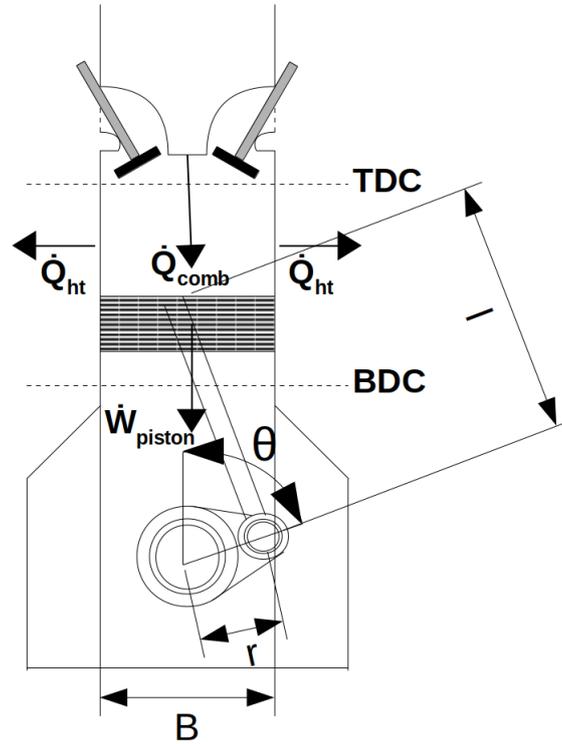
Figure 1: Diesel Engine Schematics.

It is important to highlight the physical phenomena of heat transfer between the combustion chamber and the cylinder wall. According to Stone (1999), it is possible to assume the wall temperature as a constant value, which is recommended by Stone (1999) to be set at 350 K. Then, the results are obtained by using the zero-dimensional approach mentioned before.

The values from engine speed, injection angle, inlet temperature and inlet pressure were taken from Belchior and Pimentel (2003). Whereas other properties, such as diesel density and its low heating value, were taken from Heywood (1988) as shown in Table 1.

Table 1: Operational Parameters (Belchior and Pimentel, 2003)

Property	Variable	Value
Engine Speed	N	900 rpm
Injection Angle	θ_{inj}	-13 °CABTDC
Diesel Density	ρ_{fuel}	832 kg m^{-3}
Air's Heat Capacity Ratio	γ	1.3-1.35
Stoichiometric fuel-air ratio	ϕ_{sto}	0.06817
Inlet Temperature	T_{inlet}	339 K
Inlet Pressure	P_{inlet}	1.416 bar

3. NUMERICAL MODEL

3.1 Forward Problem

According to Merker *et al.* (2005), diesel engines operate in four different strokes, with the piston moving between top and bottom dead centres: inlet, compression, combustion and exhaust. Nonetheless, this paper will be strictly concerned with the compression stroke. Thus, The First Law of Thermodynamics backs a temperature equation given by Eq. (1). Similarly, the pressure equation can be generalized from Thermodynamics. Again, focusing on the compression stroke, is obtained the Equation (2) (Heywood, 1988). To sum up, the equations have the following variables: temperature (T

in K), pressure (P, in bar), mass (m, in kg), volume (V, in m^3), heat (Q, in kJ), gas coefficient (R, in $\frac{kJ}{kg\ K}$), internal energy (u, in kJ), heat capacity ratio (γ, dimenssionless) and crank angle (θ, in °CABTDC)

$$\frac{dT}{d\theta} = \frac{\left(\frac{dQ}{d\theta}\right)\frac{1}{m} + \frac{RT}{V}\frac{dV}{d\theta}}{\frac{du}{dT}} \tag{1}$$

$$\frac{dP}{d\theta} = \frac{\gamma}{V}\left[\left(\frac{dQ}{d\theta}\right)\left(\frac{\gamma-1}{\gamma}\right) - P\frac{dV}{d\theta}\right] \tag{2}$$

The heat flux in the chamber wall can be described in Equation (3) (Heywood, 1988). The heat coefficient is described by Hohenberg (1979) as seen in Equation (4).

$$\frac{dQ}{d\theta} = hA_c\left(T - T_w\right) \tag{3}$$

$$h = 130P^{0.8}T^{-0.4}V_s^{-0.06}\left(2S\frac{N}{60} + 1.4\right)^{0.8} \tag{4}$$

The chamber area is described by Equation (5) (Heywood, 1988). The chamber volume is expressed by Equation (6) (Heywood, 1988).

$$A_c = \pi B^2 + \pi B r\left(\frac{l}{r} + 1 + \cos\theta - \sqrt{\left(\frac{l}{r}\right)^2 - \sin^2\theta}\right) \tag{5}$$

$$V = \frac{V_s}{r_c - 1} + \pi\frac{B^2}{4}\left(l + r - \left(r\cos\theta + \sqrt{l^2 - r^2\sin^2\theta}\right)\right) \tag{6}$$

Finally, internal energy in Equation (1) can be modeled using the Krieger and Borman approach (Watson and Janota, 1982), as seen in Equation (7). The system of coupled non-linear ODEs, given by Eq.(1)-(2), is solved using the Fourth Order Runge-Kutta Method.

$$u(T,\phi) = 0.692T + \left(39.17 \times 10^{-6}\right)T^2 + \left(52.9 \times 10^{-9}\right)T^3 - \left(228.62 \times 10^{-13}\right)T^4 + \left(227.58 \times 10^{-17}\right)T^5$$
$$\phi\left(-\left(5.7 \times 10^{-2}\right)T - \left(9.5 \times 10^{-5}\right)T^2 + \left(21.53 \times 10^{-9}\right)T^3 + \left(2000.26 \times 10^{-14}\right)T^4\right) \tag{7}$$

3.2 Inverse Problem

In this paper, the goal of the inverse problem is to estimate the initial conditions of pressure and temperature, assuming that pressure measurements are available during the compression stage. To perform this task, the Levenberg-Marquardt algorithm was used (Ozisik and Orlande, 2000). In this method, sought variables are estimated via nonlinear regression, whose function is given by Eq. (8)

$$S(\mathbf{x}) = |\mathbf{y} - \mathbf{f}(\mathbf{x})|^2, \tag{8}$$

where $\mathbf{y}$ represents the pressure measurements, $\mathbf{x}$ is the vector of unknowns (namely, the sought initial conditions) and $\mathbf{f}()$ is a non-linear function that maps from the set of possible initial conditions to the set of possible pressure curves. The Levenberg-Marquardt algorithm is an iterative solver designed for regression problems, whose equations are given by Eqs. (9a)-(9b) (Ozisik and Orlande, 2000).

$$\mathbf{x}_{k+1} = \mathbf{x}_k + [\mathbf{J}_k^T\mathbf{J}_k + \lambda_k\mathbf{\Omega}]^{-1}\mathbf{J}_k^T[\mathbf{y} - f(\mathbf{x}_k)], \tag{9a}$$

$$\mathbf{\Omega} = diag[\mathbf{J}_k^T\mathbf{J}_k]. \tag{9b}$$

An important aspect to be observed is that one can only expect the algorithm to converge if the first bracketed term in Eq. (9a) is invertible. To evaluate if such is the case, a sensivity analysis was performed, which concluded that both paraeters are linearly independent, so that they can be successfully estimated at the same time during the compression stroke. It is shown in Fig 2
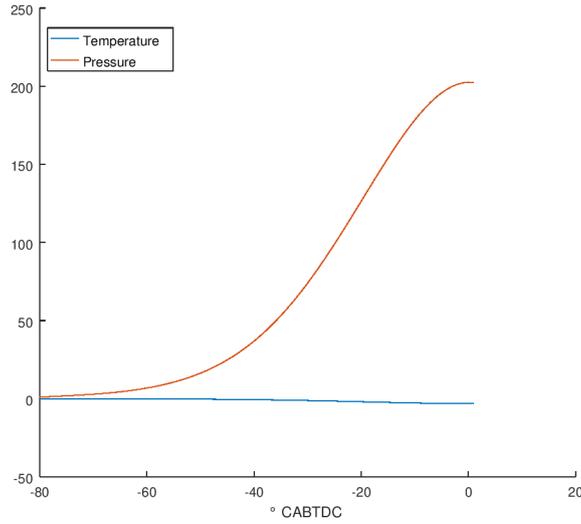
Figure 2: Sensivity analysis of temperature and pressure.

Being the initial conditions of pressure and temperature the sought parameters, the unknown vector is written as $\mathbf{x}_k = [P_{0,k} \ T_{0,k}]^T$, while the measurements vector contains the measured pressure values.

4. RESULTS AND DISCUSSION

Overall, this paper seeks to evaluate robustness of the proposed methodology and to verify the computer code created. Therefore, a numerical experiment was conceived where synthetic measurements of pressure were assumed be available. These measurements were obtained by solving the forward problem with preference P_0 and T_0 and then adding Gaussian noise with zero mean and standard deviation $\sigma_y = 0.2$ bar to these pressure values, in order to mock the uncertainties of a real scenario.

To provide the Levenberg-Marquardt method with an initial estimate of the exact vector $\mathbf{x}$ was multiplied by 0.9, yielding a value of $\mathbf{x}_0 = [1.2744 \ \ 305.10]^T$. The stop criteria for the algorithm is to perform until the ratio of the iteration's increment of the vector (Δx) and the initial vector $(\mathbf{x}_0)$ reaches a value of 10^{-6}. Furthermore, on average, it led into 100 iterations to meet the stop criteria. The results can be seen in Fig. 3a, and one can observe that the exact and estimated pressures present a good fit. Furthermore, the numerical values considered can be observed in Tab. 2.

In terms of computacional cost, the present research has shown a fast response during the inverse analysis by finishing the Levenberg-Marquard algorithm in 143.46 seconds with 179 iterations using a computer with a CPU of 1.80 GHz with 4 cores and 8 threads. In fact, it is important to highlight how inverse analysis tend to have a huge computacional cost, which the opposite is shown here.

Due to the presence of Gaussian noise in the data, the residuals are expected to be of the same nature of the if the inverse problem is correctly solved. Firstly, a homoscedasticity test, which is done through a residual plot as seen in Fig 3b, it can be observed that the obtained residuals oscillate around zero, with amplitude of the same order of σ_y providing evidence that information from the date was successfully obtained. Then, a Q-Q plot of the residuals was made, as seen in Fig. 4. Also, Wilson-Shapiro test was performed returning a value of 0.38232. Therefore, the residuals are indeed follow a normal distribution.

Table 2: Estimated values for pressure and temperature.

	P_0 [bar]	T_0 [K]
Exact	1.4160	339.0000
Initial	1.2744	305.1000
Estimated	1.4564	341.6295
Relative Error	2.8531 %	0.7756 %

It is important to analyse the behaviour of the algorithm when some of the fixed parameters are slightly changed as seen in Tab. 3. As seen, the parameters of heat coefficient (h) and the derivative of internal energy in terms of temperature $\left(\dfrac{du}{dT}\right)$ do not display a huge sensitivity on the accuracy of the model outcome. However, parameters such as wall temperature (T_{wall}) and heat capacity ratio (γ) does show a sensitivity for convergence using the Levenberg-Marquardt algorithm when the two parameters are slightly changed. When testing for different values of γ and T_{wall}, the algorithm failed to

converge. This indicates that, although the proposed approach is regarding uncertainties in h and $\dfrac{du}{dT}$. The values of γ and T_{wall} must be very precisely known to avoid convergence setbacks.

Table 3: Numerical values for pressure and temperature.

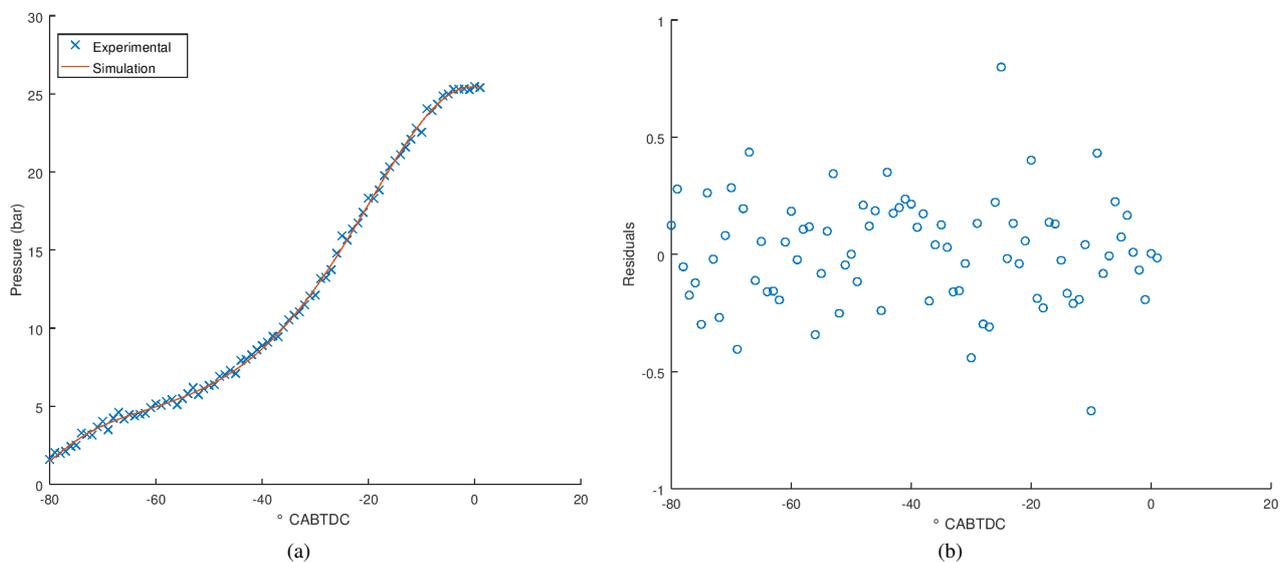|	P_0 [bar]	P_0 relative error	T_0 [K]	T_0 relative error	Shapiro-Wilk
105% h	1.453061	2.6173%	341.3827	0.7029%	0.70592
95% h	1.374388	2.9387%	336.2091	0.8233%	0.89263
105% $\dfrac{du}{dT}$	1.510352	6.6633%	345.0145	1.7742%	0.99782
95% $\dfrac{du}{dT}$	1.374616	2.9226%	336.2104	0.8229%	0.44653

(a)

(b)

Figure 3: Results of the inverse analysis: a) comparison between exact and estimated pressure; and b) respective residuals.
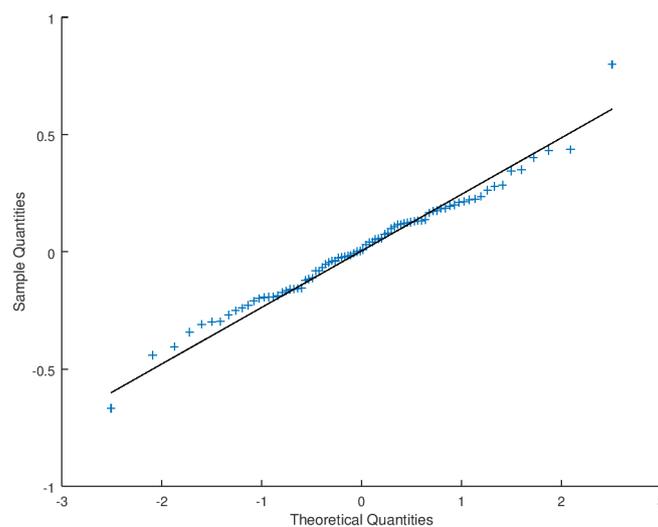

Figure 4: Q-Q Plot of Residuals.

Since the mathematical model of this research also includes temperature during the compression stroke, a performance of the temperature curve was made in order to discuss how powerful the inverse analysis is for a curve that belongs to the system of ODEs presented on this study. Then, it was plotted a temperature curve using the initial conditions from the experimental data, which is compared with the temperature curve using the initial conditions resulted from the inverse analysis as seen in Fig 5a. Furthermore, to compare the error between the curves it was plotted the difference between

them, as seen in Fig 5b. In fact, it is possible to stress how effective is the comparison when the crank angle is at -60°and the difference between the curves starts to converge to zero.

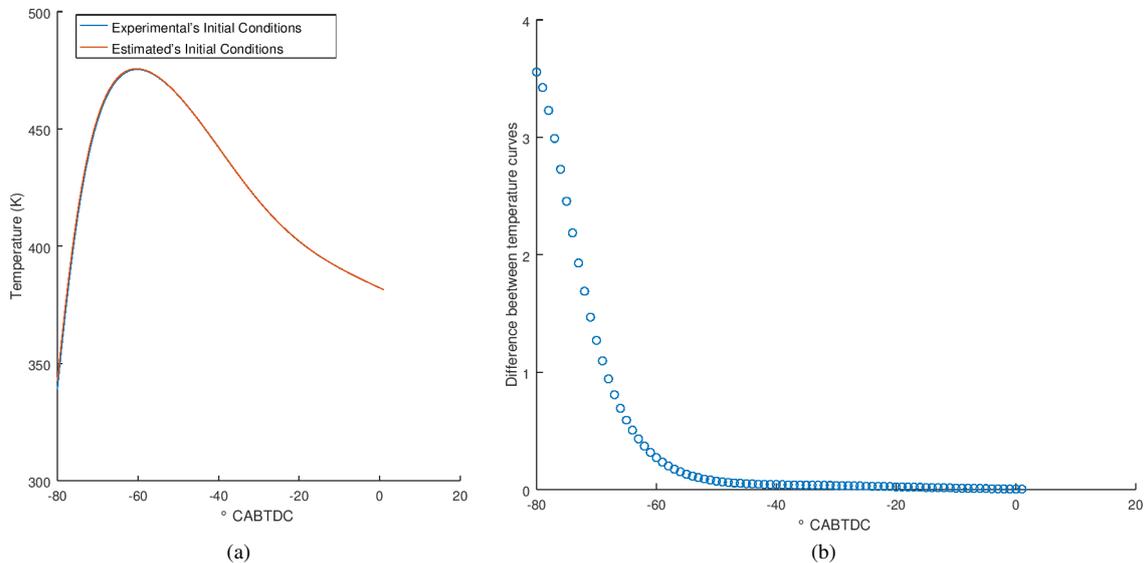(a)   (b)

Figure 5: Results of the temperature curve: a) comparison between experimental and estimated initial conditions; and b) difference between temperature curves.

5. CONCLUSIONS

This paper proposed a numerical analysis to recover the initial conditions of pressure and temperature of a CFR diesel engine for cetane testing backed by the standard ASTM D613. This process has been carried through by means of an inverse analysis, using the Levenberg-Marquardt algorithm. The method presented a excellent performance, achieving convergence of the initial conditions for Pressure and Temperature with an absolut error of 2.8531 % 0.7756 %.

Also, it is important to highlight that some tests were made trying to check the sensivity of the algorithm where it was performed a Shapiro-Wilk test to check if the residuals fit a normal distribution when slightly changing some parameters, such as heat coefficient (h), the derivative of internal energy in terms of temperature $\left(\dfrac{du}{dT}\right)$, wall temperature ($T_{wall}$) and heat capacity ratio (γ). Then, via Shapiro-Wilk test, the parameters of h and $dudT$ do not display a huge sensity when slightly changed. However, T_{wall} and γ did show a sensivity on the algorithm when slightly changed.

To conclude, similar studies can be done with this problem by choosing different parameters to be obtained via inverse analysis such as wall termperature, air-fuel ratio and heat capacity ratio. Moreover, the inverse analysis can be done through metaheuristc approaches, such as genetic algorithm, simulated annealing and tabu search. Also, it will be interesting to not just focus on compression stroke and perform an analysis on the four strokes. Furthermore, more experimental data would be very useful using different engine geometries and operational parameters.

6. ACKNOWLEDGEMENTS

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8. RESPONSIBILITY NOTICE

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