Comparison of two thermodynamic combustion models

A Sabau

Maritime University of Constanta, 104, Mircea cel Batran, St.9000663, Constanta, RO

adrian.sabau@cmu-edu.eu

Abstract. The paper aims at making a comparison between two models of the process of thermodynamic combustion, the fuel rate model and the Wiebe's function model, used for the prediction of the engine performance. The paper shows a practical method that enables a basic calibration of the constants encountered in the mathematical models when there are no concrete experimental data for the specified engines, but there are data for similar engines. The models have opposite starting hypotheses in the frame of the combustion process modelling and there is the advantage of a large number of well documented case studies in the reference literature. Both models use the Annand and Pflaum approximations for the heat release assessment, that have particular relations for the piston, the linear cylinder and the cylinder cover. The chemical mechanism use stoichiometric reactions taking into account the dissociation.

1. Introduction

A major problem of the design stage of the compression ignition engine is represented by the prediction of the engine performance. This task is difficult to accomplish since the number of parameters is rather large and the links between them are non-linear. The same happens to all the other processes that take place in the engine, and especially with the combustion process which is the most complex of them all due to the large number of phenomena that take place simultaneously.

Many combustion models have been developed, most of them being very complex since they require a large number of parameters. Consequently, it becomes impossible to apply this type of model in the early stage of the design because most of the initial data are not known.

The paper presents a theoretical model of the entire cycle for a compression ignition engine by using two combustion models. For this model the author has developed an original computing code, the main feature being the minimum number of the initial parameters taken into consideration.

The theoretical approaches are based on the models of thermodynamic combustion and all other processes are treated in a global manner so that the entire cycle can be actually simulated.

2. Theoretical backgrounds

The inlet process is described using the First Law of Thermodynamics for an open system, the continuity equation and the equations of the pressure of steady flow from orifices.

These equations were solved using different approaches in the flow equation and thermodynamics constants. Finally we can obtain pressure p_{in} and temperature T_{in} at the theoretical end of the inlet process:

$$p_{in} = \frac{p_s}{\sigma} \left(1 - \frac{n^2}{1800 \frac{n_a}{n_a - 1} \frac{RT_s}{M_{aer}}} \frac{\left(\frac{\varepsilon - \mu\rho}{\varepsilon - 1}\right)^2}{\phi^2 \left(fm\_Vs \cdot n\right)^2} \right)^{\frac{n_a}{n_a - 1}} ,$$
(1)

$$T_{in} = T_s \frac{p_{in}}{p_s} \frac{\varepsilon}{\varepsilon - 1} \left[1 + \frac{\rho p_{out} T_s \nu \, p_{in}}{p_s^2 T_{out} (\varepsilon - 1)^2 \theta \, n_a} \cdot \left(\varepsilon + (n_a - 1)(\varepsilon - 1)\sigma - \frac{p_{out}}{p_{in} \rho} \right) \right],$$ (2)

T_s ; p_s inlet air parameters, T_{out} ; p_{out} exhaust gas parameters, ε compression ratio, θ ratio of temperature increase, ρ scavenge coefficient, ϕ debit and velocity coefficient flow in inlet valve, fm_V_s ratio of section time and piston displacement, $\mu = \dfrac{p_{out}}{p_{in}} \dfrac{T_{in}}{T_{out}}$, ν coefficient of inertial inlet, n_a isentropic index, n speed engine [1] .

The compression process may be calculated using the first law of thermodynamics for a closed system.

In order to calculate the changes for p and T, we discretize the volume $dV = V_{j+1} - V_j$ and for every small step we ar use the First Law of Thermodynamics. For this approach we can apply the First Law of Thermodynamics in the form:

$$dQ = \Delta E + dW ,$$ (3)

where dQ is the heat transfer to the cylinder walls.

If the cylinder wall temperature is T_w and the exposed surface area is A, then the heat transfer is:

$$\frac{dQ_t}{dt} = \alpha_c A(T_{mj} - T_w) + \alpha_r A(T_{mj}^4 - T_w^4) \qquad \left[\frac{j}{s} \right]$$

$$\frac{dQ_t}{d\alpha} = \left[\alpha_c A(T_{mj} - T_w) + \alpha_r A(T_{mj}^4 - T_w^4) \right] \frac{1}{6n} \quad \left[\frac{j}{\deg} \right],$$ (4)

α_c convective heat transfer coefficient, α_r radiative heat transfer coefficient.

Anand, Pflaum, Woschni, Eichelberg et. al proposed formula for heat transfer. We used Annand and Pflaum relations [2].

$$\text{Annand:} \begin{cases} \alpha_c = a \dfrac{k}{D} \text{Re}^b \\ \alpha_r = c \end{cases},$$ (5)

$$\text{Pflaum:} \begin{cases} \alpha_c = (k_1 + k_2 \dfrac{p_s}{p_{in}})(k_3 + k_4 e^{k_5 \overline{w_p}}) \sqrt{pT} \\ \alpha_r = \sigma_B c_r \end{cases},$$ (6)

Re Reylonds number, K thermal conductivity, $\overline{w_p}$ mean piston velocity, σ_B Stefan Boltzman constant, $k_1, .. k_5, c_r$ coefficients of Pflaum formulae regarding different area type, a, b, c coefficients of Annand's formula.

For a step of time/angle the pressure change from p_j to p_{j+1}. If the volume change is small, the "work" term can be given approximately by

$$dW = pdV = \frac{p_j + p_{j+1}}{2} \left(V_{j+1} - V_j \right).$$ (7)

For the volume we used the approaches:

$$V_j = \frac{V_s}{\varepsilon - 1} + \frac{V_s}{2}\left[\left(1 - \cos(\alpha_j)\right) + \frac{\lambda}{4}\left(1 - \cos(2\alpha_J)\right)\right],\tag{8}$$

which are the first two terms of a Taylor series, where, $\lambda = \dfrac{S}{2L}$, S and L is the piston stroke and the connecting rod length.

Equation (3) cannot be solved analytically and a numerical solution must be sought. In principle this requires the estimation of T_{j+1} to obtain p_{j+1} at which step of time/angle:

$$p_{j+1} = \frac{V_j}{V_{j+1}}\frac{T_{j+1}}{T_j}p_j.\tag{9}$$

This pressure is substituted in the rearranged equations of the First Law:

$$e = \Delta E + dW - dQ_t.\tag{10}$$

A solution is obtained when $e \to 0\,(|e| < .001)$. The numerical scheme used is the Newton-Raphson method. In this method if $(T_{j+1})_{q-1}$ is the estimated value of T_{j+1} this has the expression [3]:

$$\left(T_{j+1}\right)_q = \left(T_{j+1}\right)_{q-1} - \frac{e_{q-1}}{MCv[(T_{j+1})_{q-1}]}.\tag{11}$$

For a volume change dV the conditions at moment j the beginning of the step will be equal to the conditions at the state $j+1$ at end of the previous volume step. The first estimate of T_{j+1} may be obtained by assuming an isentropic change from the state conditions at T_j thus:

$$T_{j+1} = T_j\left(\frac{V_j}{V_{j+1}}\right)^{\frac{\Re}{Cv(T_j)}}.\tag{12}$$

The internal energy $E(T_j)$ and the specific heats $Cv(T_j)$ are calculated used the gas composition and temperature (we used a polynomial IV degree expression).

The injection, ignition and expansion, the most important processes in the engine cycle will be treated simultaneously.

The ignition reaction was modelled using the stoichiometric equation:

$$\begin{cases} C + O_2 = CO_2 \\ H_2 + \dfrac{1}{2}O_2 = H_2O, \\ S + O_2 = SO_2 \end{cases}\tag{13}$$

and reaction of CO_2 dissociation,

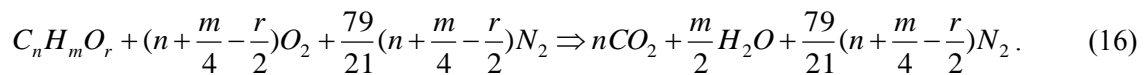$$\delta CO_2 \rightarrow \delta CO + \frac{\delta}{2} O_2 \,, \tag{14}$$

where $K_{Pco} \sqrt{\dfrac{p}{v}} = \dfrac{1-\delta}{\delta \left(\dfrac{1}{2}\delta\right)^{\frac{1}{2}}}$, and $\delta = \sqrt[3]{\dfrac{2}{K_{Pco}^2} \dfrac{v}{p}}$, or $\delta = \delta' \sqrt[3]{\dfrac{v}{p}}$, using : $\begin{cases} v = v + \dfrac{1}{2}v \cong 1 \\ \delta' \cong 10^{-7}(T-1400)^2 \end{cases}$ [3].

The mass of *CO* obtained from dissociation is too small and we considered its mass as being negligible but it is very important for heat balance when the temperature raises over 1400 K.

$$dQ_d = \delta \cdot dm_{CO_2} \cdot Q_{CO} \ [\text{j}], \tag{15}$$

where Q_{CO}=279231 [kj/kg].

The fuel was approximated as a chemical pure substance having the formula: $C_nH_mO_r$. This approach allowed us to calculate the products of combustion according to the reaction:

$$C_nH_mO_r + (n + \frac{m}{4} - \frac{r}{2})O_2 + \frac{79}{21}(n + \frac{m}{4} - \frac{r}{2})N_2 \Rightarrow nCO_2 + \frac{m}{2}H_2O + \frac{79}{21}(n + \frac{m}{4} - \frac{r}{2})N_2 \,. \tag{16}$$

The ignition delay time was calculated with the formula proposed by Baert [4]

$$\tau_{aa} = \tau_{ao} + k_1 p^{-n1} \exp\left(\frac{E}{\Re T}\right) + k_2 p^{-n2} \ [\text{ms}], \tag{17}$$

where $\tau_{ao} = 0.36$, k_1=1.154x10^{-4}, $k2$=2550, $n1$=0.75, $n2$=2.45, $E/\Re = 9495$.

The injection law considered was a linear one, but supplementary parabolic and polynomial (second degree) have been taken into account.

The fuel instantaneous vaporisation has also been treated only from the energetic point of view:

$$dQ_v = \left[Lv + c_l(T_s - T_l)\right]dm_{inj} \ [\text{j}], \tag{18}$$

whit *Lv* latent vaporisation heat; c_l specific heat; T_s vaporisation temperature; T_l temperature of fuel.

During the combustion period, the heat release was obtained by using two models:

- the Wiebe functions model,
- the fuel rate Whitehouse-Way model.

The first model proposes an empirical formula for the rate of heat release based on the analysis of the experimental rate of heat release diagram according to the expression:

$$\frac{dQ_b}{d\alpha} = a_p \frac{\Delta Q_{pr}}{\Delta \alpha_p} (M_{pr}+1)\left(\frac{\alpha}{\Delta \alpha_{pr}}\right)^{M_{pr}} e^{-a_p\left(\frac{\alpha}{\Delta \alpha_{pr}}\right)^{M_{pr}+1}} + a_d \frac{\Delta Q_d}{\Delta \alpha_d}(M_d+1)\left(\frac{\alpha}{\Delta \alpha_d}\right)^{M_d} e^{-a_d\left(\frac{\alpha}{\Delta \alpha_d}\right)^{M_d+1}} \,. \tag{19}$$

For the automatic calibration of the constants we used experimental correlations [5]. This expression takes into account dependencies of constants to the timing injection, considering that, this is the most important parameter. Usually $a_p=a_d=6.9$.

The numeric calculation expressed heat release in a small step according to the formula:

$$dQc = (dQ_b d\alpha)m_{inj} \ [\text{j}], \tag{20}$$

This formula permits the heat release calculation for any time step of the calculus.

The second method calculates heat release using two expressions for the fuel preparation and reaction rates [6].

The fuel preparation rate is given by:

$$\frac{dm_{pr}}{d\alpha} = km_{inj}^{1-x}m_u^x p_{O_2}^m \ \ [\text{kg/deg}], \tag{21}$$

the reaction rate by:

$$\frac{dm_b}{d\alpha} = \frac{60k' p_{O_2}}{n\sqrt{T}} e^{\frac{-E}{T}} \int \left(dm_{pr} - dm_b\right) [\text{kg/deg}]. \tag{22}$$

m_{inj} [kg] total mass of injected fuel, m_u [kg] mass of unburned fuel; $m_u = m_{inj} - \int (dm_{pr})d\alpha$, k and m constants, p_{O_2} [bar] partial pressure of oxygen, E [j] activation energy, k' constant, n engine speed.

The numeric calculations using the fuel rate model consider that:

$$(m_{inj})_{i-1} = \sum_1^{n-1} \frac{dm_{inj}}{d\alpha}\Delta\alpha \ . \tag{23}$$

Similarly, the total fuel prepared and burnt in the cylinder is given by:

$$(m_{pr})_{i-1} = \sum_1^{i-1} dm_{pr}\Delta\alpha \ , \tag{24}$$

$$(m_b)_{i-1} = \sum_1^{i-1} dm_b\Delta\alpha \ . \tag{25}$$

In principle average values of m_{inj} and m_u for step would be the logical values, but this demands a knowledge of the conditions at the end of the step, which can only be obtained by an iterative procedure. If the change in the values during the step is small enough, relative to the absolute values, which is usually true for the step size used in these calculations, the initial values could be used.

For the first step of the process, when m_{inj} and m_u are very small, this condition is not valid and use of initial values alone would underestimate preparation rate. For this reason, as m_{inj} is usually known and specified as data, the final value of m_{inj} for the step may be used [6].

Then in equation (21):

$$m_{inj} = (m_{inj})_i \text{ and } m_u = (m_{inj})_i - (m_{pr})_{i-1} \ , \tag{26}$$

gives the preparation rate during the step as:

$$\left(\frac{dm_{pr}}{d\alpha}\right)_i = k\left(m_{inj}\right)_i^{1-x}\left[\left(m_{inj}\right)_i - \left(m_{pr}\right)_{i-1}\right]^x p_{O_2}^m \text{ [kg/deg]}, \tag{27}$$

and the total fuel prepared

$$\left(m_{pr}\right)_i = \left(m_{pr}\right)_{i-1} + \left(\frac{dm_{pr}}{d\alpha}\right)_i \Delta\alpha \text{ kg].} \tag{28}$$

For the fuel burnt during this step we use the reaction rate equation (22)

$$\frac{dm_b}{d\alpha} = \frac{60k' p_{O_2}}{n\sqrt{T}} e^{\frac{-E}{T}} \left[\left(m_{inj}\right)_i - \left(m_b\right)_{i-1}\right] \text{ [kg/deg].} \tag{29}$$

The fuel burnt including that burnt in the step under consideration is now:

$$\left(m_b\right)_i = \left(m_b\right)_{i-1} + \left(\frac{dm_b}{d\alpha}\right)_i \Delta\alpha \text{ [kg].} \tag{30}$$

If $\left(m_b\right)_i < \left(m_{pr}\right)_i$ the burning rate is lower due to the conditions in cylinder, then the fuel consumed in the step is assumed to be:

$$dm_c = \left(m_b\right)_i \Delta\alpha \text{ [kg].} \tag{31}$$

If $\left(m_b\right)_i > \left(m_{pr}\right)_i$, the burning rate is higher than the assumed rate, the process is controlled by the rate of preparation and fuel consumed in the step is:

$$dm_c = \left(m_{pr}\right)_i \Delta\alpha \text{ [kg].} \tag{32}$$

Using the mass of fuel consumed in each step of the cycle calculation we may determinate the value of the heat release dQ_c:

$$dQ_c = dm_c\, Q_i \text{ [j],} \tag{33}$$

where Q_i is the lower specific heat value of the fuel.

The first law of thermodynamics for combustion and expansion process in accord whit the rearranged formula is:

$$e = \left[E_{j+1}\left(T_{j+1}\right) - E_{j+1}\left(T_s\right)\right] - \left[E_j\left(T_j\right) - E_j\left(T_s\right)\right] + dW - dQ_c - dQ_t - dQ_v - dQ_d, \tag{34}$$

where T_s is the reference temperature for the chemical reaction and the others terms in the equation has the form previously expressed.

A solution is obtained when $e \rightarrow 0\,(\left|e\right| < .001)$. The numerical method used for solving the first law expression is Newton-Raphson. According to this method if $(T_{j+1})_{q-1}$ is the estimated value of T_{j+1} it is possible to conduct an iterative scheme to solve the equations and this is done by the expression:

$$\left(T_{j+1}\right)_q = \left(T_{j+1}\right)_{q-1} - \frac{e_{q-1}}{MCv[(T_{j+1})_{q-1}]} \; . \tag{35}$$

In this case the pressure and the temperature at the end of the step have the following formula:

$$p_{j+1} = \frac{m_{j+1}}{m_j} \frac{V_j}{V_{j+1}} \frac{T_{j+1}}{T_j} p_j \; , \tag{36}$$

$$T_{j+1} = T_j \left(\frac{V_j}{V_{j+1}}\right)^{\frac{\Re}{Cv(T_j)}} + \frac{dQ_c}{m_j C_v\left(T_j\right)} \; . \tag{37}$$

The expansion stroke was solved simultaneously with the combustion process as a continuation of the last one with $dQ_c=0$.

The exhaust process was globally treated and the corresponding pressure was constant (the initial parameter). The temperature of the residual gases which was initially approximated was calculated simulating the expansion as a polytropic process with a constant exponential coefficient, ending at the inlet pressure. The temperature was corrected until the imposed error was less then 1%.

Mechanical efficiency is a very important parameter for the estimation of the engine performance. The lost friction power was modelled based on Millington & Hartles and Whinterbone & Tenant's expresions [7].

Approaches for cycle calculation. The inlet and exhaust strokes have 180 revolution degrees and an imposed pressure value sets as initial data. The injection timing is initially set and has a constant value. The computation has as goal to obtain the engine dimensions according to the imposed engine power and the correction of the necessary residual gas temperature or to estimate the output power for the imposed engine dimensions. The optimization consists in variating the initial parameters so that in the end we obtain the performance indicators.

Numerical simulation was done by using an original code developed in Matlab MatWorks environment. Matlab has an impressive library of functions for every part of the simulation program: mathematical functions, functions for solving transcendent equations or differential equations, functions for manipulating data and for graphical representations. The code is developed in an open architecture, only the initial data imput has a minimal interface for data protection and flexibility. The rest of the program is in fact a collection of functions called by a main routine.

The data result is not filtered and for this reason it is mandatory to interpret results with additional attention. It is possible to obtain a non-physical value duet o the numerical algorithm and cut-off errors. To facilitate the data comparison between the result values and the experimental data the code has a library of interpolation function.[8].

3. Results

Results of the cycle calculations are presented using the diagrams below. Figure 1 is shown the cycle diagram (p(α)) for a four stroke direct injection AT 25 Sulzer engine.
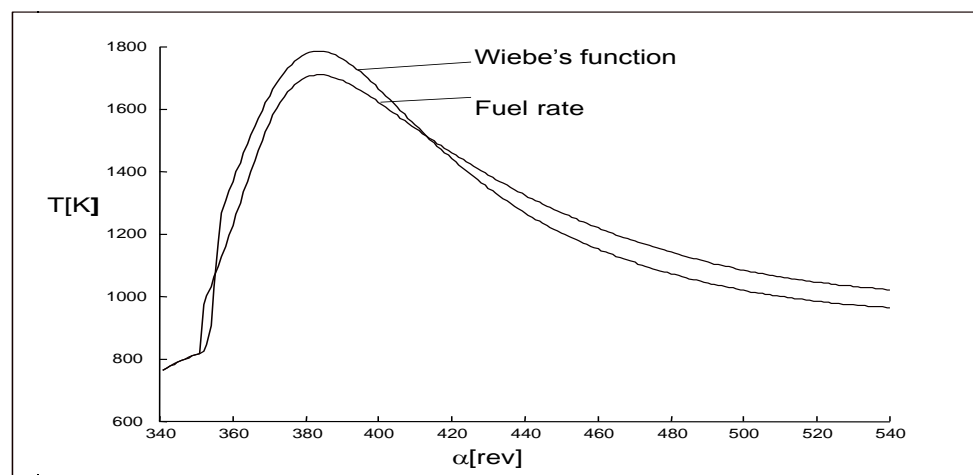
In Figure 2 to 6 we present comparative results calculation based on Wiebe's function combustion model and fuel rate Whitehouse-Way's model by using Annand's formula for the heat transfer .
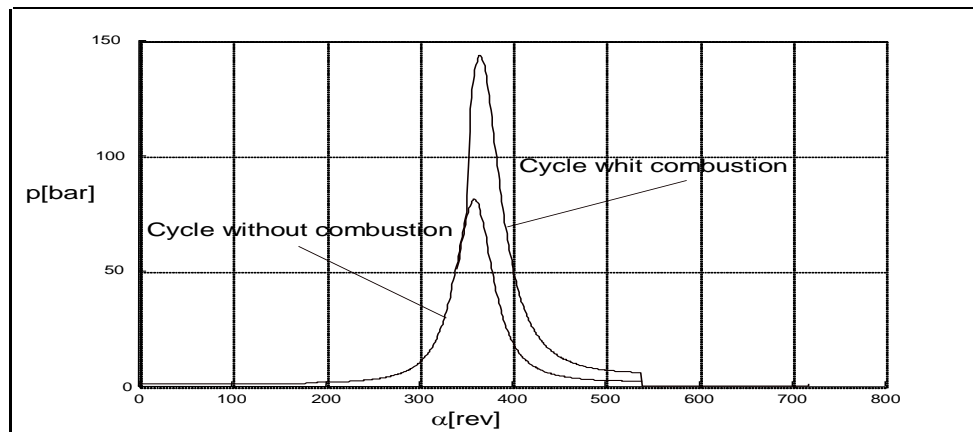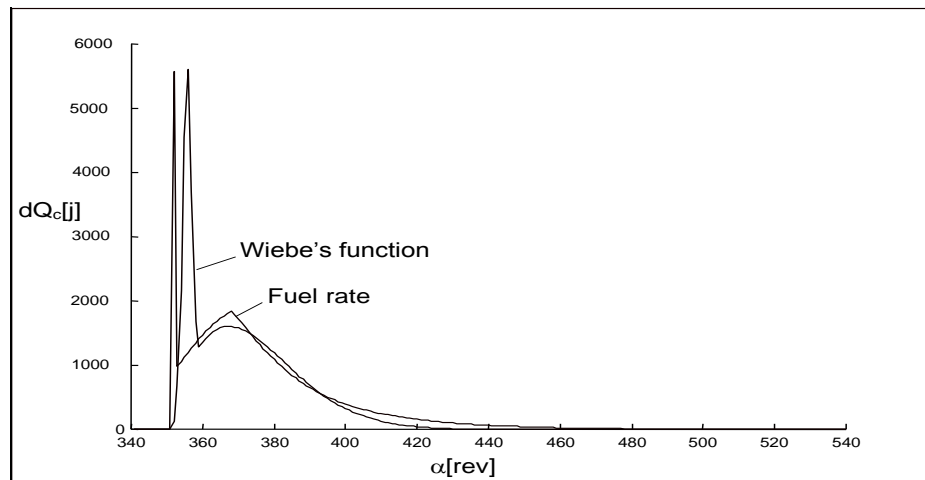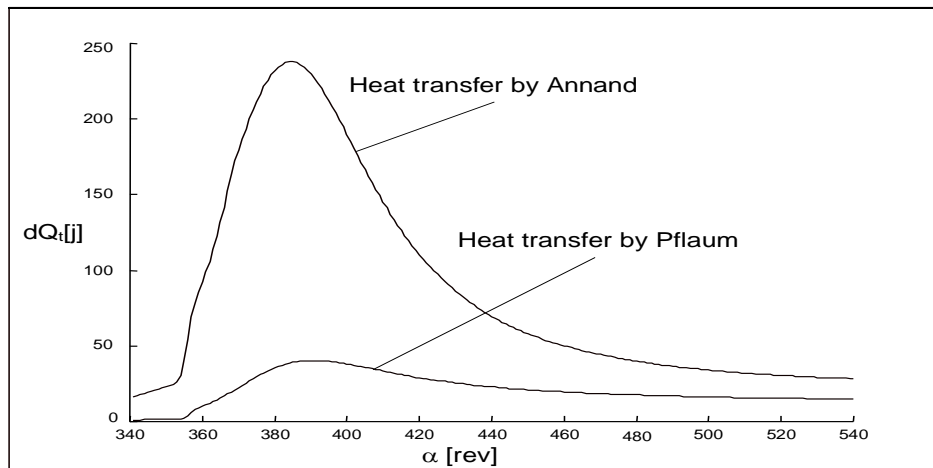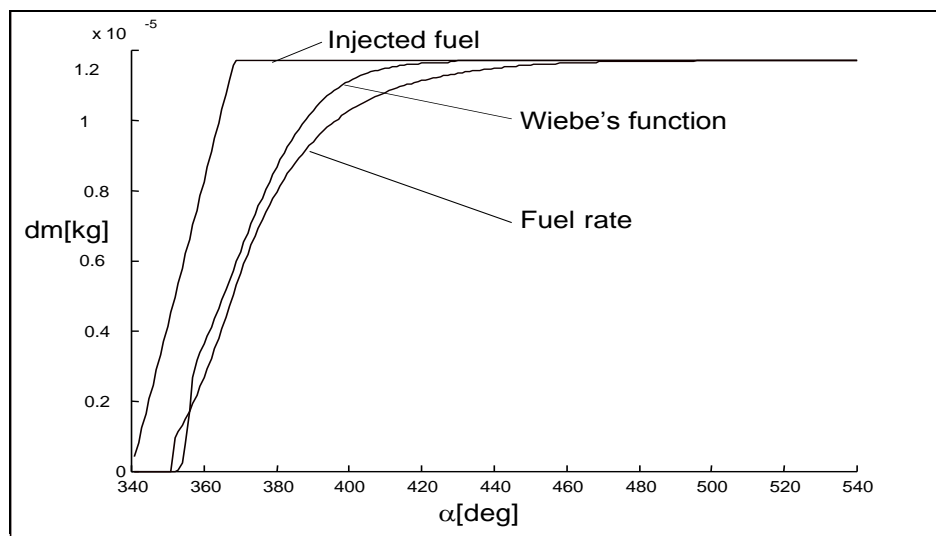
Figure 1 p(α) diagram
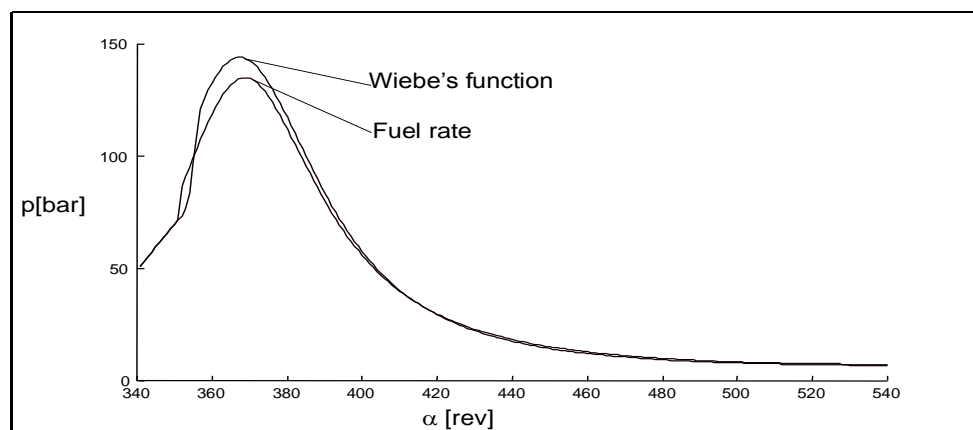
**Figure 2**. p(α) combustion and expansion

**Figure 3**. T(α) combustion and expansion

Figure 4. Heat release

Figure 5. Heat transfer

Figure 6 Mass of fuel burnt and injected

The heat transfer pattern for both methods Annand and Pflaum formulations is presented in Figure 5. Pflaum formula gives a small heat transfer rate and, consequently, not satisfactory results. This is the reason why we used only Annand's formula for the calculus.

The code results were verified whit experimental data p(α) diagram at 1000 rev/min and 100% (nominal regime). The real indicated diagram (Figures 7 and 8) was available for this checking which was compared with the computed indicated diagram.
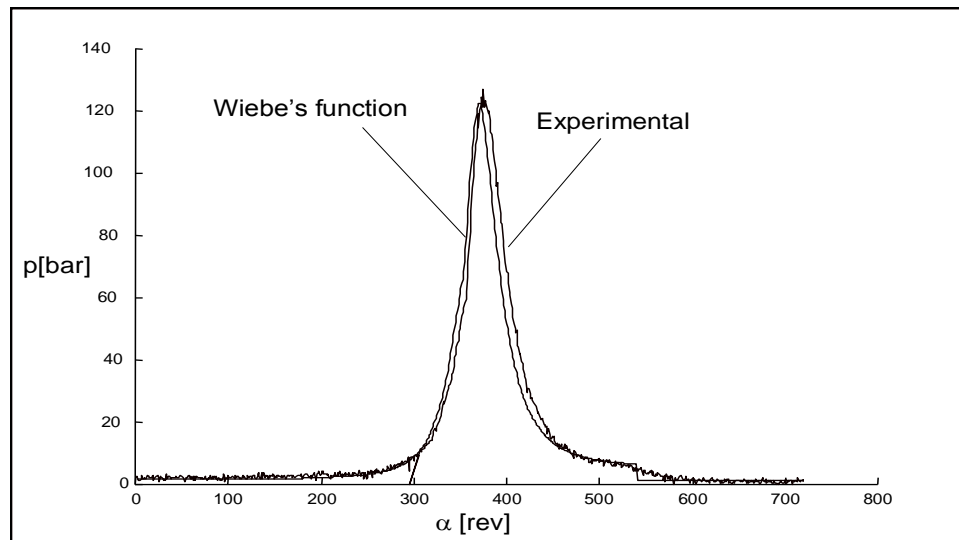
Figure 7. Indicated Wiebe's function and experimental diagram.
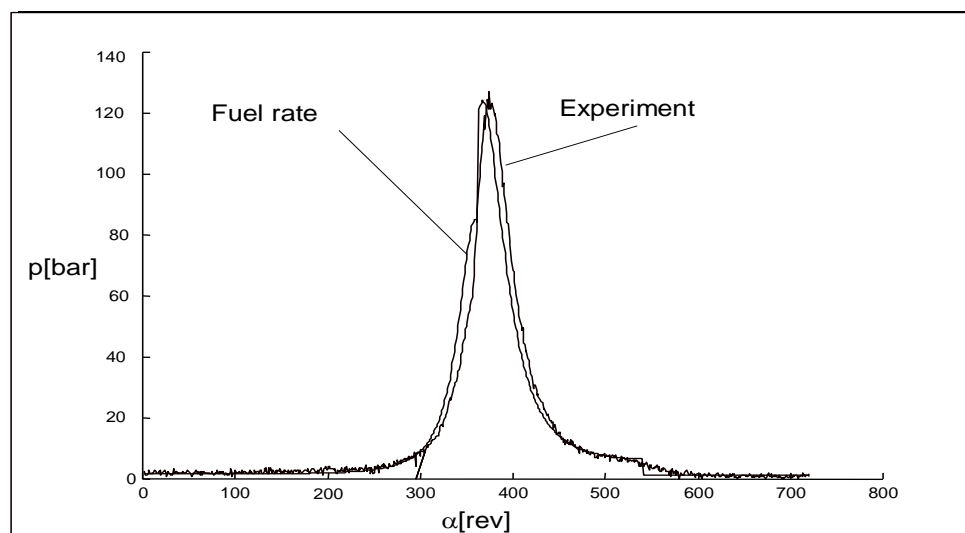
Figure 8. Indicated fuel rate and experimental diagram.

The numerical calculus with automatic calibrated Wiebe's function offered a satisfactory match between the diagram patterns. We must underline on the moderate differences of the amplitudes. The percentage errors are bot maximum 2% for pressure, 1% for power and 1.5% the fuel consumption.

For the fuel rate model the result is not so good, since the percentage errors are of maximum 4.3% for pressure, 2% for power and 1.5% for the fuel consumption. In addition, the shape of the diagram is slightly different and the pressure peak is not in the same position.

4. Conclusions

The models used for the combustion process are enough accurate for the assessment of the performance parameter (power, efficiency and fuel consumption) for a compression ignition engine at nominal regime.

The Wiebe's function combustion model is more flexible than the fuel rate combustion model and offers a higher accuracy. The flexibility and accuracy of this model is based on a larger number of constants that must be set up as initial data. Instead the calibration of constants is a very difficult task. With a good calibration the model may offer good predictability for regimes close to the nominal one. By using Wiebe's function and proper experimental data it is possible to model any regime, but with limited accuracy and predictability.

The fuel rate combustion model has a smaller number of constants and it offers a quick solution, but with lower precision. Fuel rate models have very limited flexibility and predictability.

The code obtained from the present study is a useful tool in the early stages of design. It has the capacity to predict the running parameters and performance indicators of the compression ignition engine. The precision of the calculus depends on the initial data and can be improved if there are calibration data for that particular engine.

Even if the numerical results are accurate enough it is not possible to immediately select the final construction solution. We can only make a global evaluation and indicate the optimization directions which should be followed because the code involves many simplified hypotheses, empirical constants in the mathematical expressions and a minimum of initial parameters (these are good for the design stage but prove insufficient for a final optimal solution).

The present theoretical approaches offer appropriate solutions for the nominal regime but only satisfactory solutions for the other engines. This observation underlines on the fact that some initial parameters are not constant and are not optimal for the partial engine loads.

References

[1]   Arama, C. Grunwald B. 1966 *Motoare cu ardere interna. Procese si caracteristici* (Editura Tehnica Bucuresti)

[2]   Benson R.S. Whitehouse N.D. 1983 *Internal combustion engine* (Pergamon Press London)

[3]   Buzbuchi N Manea L Dinescu C 1997 *Motoare navale. Procese si caracteristici* (Editura Didactica si Pedagogica Bucuresti)

[4]   Dugal, V.K. Kuoo T.W. Mukerjee A., Singhal A.K. 1985 Three-dimensional modeling of in cylinder processes in DL Diesel Engines (*SAE)* Paper 840227

[5]   Heywood J.B. 1988 *Internal Combustion Engine Fundamantals* (McGraw-Hill Book Company)

[6]   Ramos J.I. 1989 *Internal Combustion Engines Modeling* (Hemisphere Publishing Corporation, New York)

[7]   Winterbone, D.E., Tennant, D.W.H. 1981, The Variation of Friction and Combustion Rates During Diesel Engine Transients (*SAE)* Paper 810339

[8]   Oanta E. Danisor A. Tamas R. 2016 *Study regarding the spline interpolation accuracy of the experimentally acquired data* (*ATOM VIII Constanta*) 1001007 doi: 10.1117/12.2242996