

## SIMPLIFIED CALCULATION OF COMBUSTION PROGRESS IN THE IC ENGINE

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**Summary.** A simplified method for MFB (Mass Fraction Burnt) determination on the basis of Energy Conservation Law has been presented in the paper. At first, cumulative heat as a function of the crank angle is computed as result of solving the mentioned law. Next, the cumulative heat after normalizing can be treated as the MFB function. Additionally, computation of the specific heat  $c_p/c_v$  ratio has also been conducted and the obtained results lead to the conclusion that accuracy in determining the  $c_p/c_v$  does not significantly influence the shape of the normalized MFB profile. Following the presented computational method, combustion phases 0-10%MFB and 10-90%MFB are also charged with a marginal error.

**Key words:** combustion engine, heat release rate, MFB.

### INTRODUCTION

Results from several works [1,2,3,4,5] concerning modeling 3-D combustion process in the internal combustion (IC) reciprocating engine with the aid of sophisticated methods including CFD technique lead to the conclusion that a simplified analysis based on empirical data from this combustion process can be sufficient for scientific purposes. However, there are also problems with this analysis particularly touching measurement methods for the TDC (Top Dead Centre) determination and in-cylinder pressure signal processing [6,7,8,9,10]. The simplified method for determining combustion progress in the IC engine is based on the Energy Conservation Law. Thus, the heat released during fuel combustion in the internal combustion engine can be described with the following equation on the basis of this principle:

$$\delta Q_{ch} = dU_s + \delta Q_{ht} + dW + \sum h_i dm_i, \quad (1)$$

where:

$\delta Q_{ch}$  – heat released from combustion,

$dU_s$  – internal energy of the fluid filling the engine cylinder,

$\delta Q_{ht}$  – heat transferred to the engine walls,

$dW = pdV$  – work done by the fluid to the environment,

$\sum h_i dm_i$  - crevices losses in energy.

The internal energy increment considered as total differential from a product of mass  $m$  and the specific heat  $c_v$  and temperature  $T$  of the working fluid can be expressed by the equation:

$$dU_s = d(mc_v dT) = mc_v dT + mT dc_v + c_v T dm = mc_v dT + c_v T dm. \quad (2)$$

Assuming that the  $c_v$  is constant and there is no mass transfer out of the closed cylinder space  $dm_i = 0$ ,  $dU_s$  can be determined as follows:

$$dU_s = mc_v dT. \quad (3)$$

Hence, after rearranging the equation (1), its form is obtained for the net heat released  $\delta Q_{net}$ , which is not influenced by heat losses  $\delta Q_{ht}$  to cylinder walls.:

$$\delta Q_{net} = \delta Q_{ch} - \delta Q_{ht} = dU_s + d. \quad (4)$$

Next, taking the differential form of the equation of state as follows

$$V dp + p dV = m R dT. \quad (5)$$

then, rearranging it to the form:

$$mc_v dT = \frac{c_v}{R} (V dp + p dV), \quad (6)$$

then, substituting it to the equation (3) and then to the equation (4) we finally obtain the equation (7):

$$\delta Q_{net} = \left( \frac{c_v}{R} \right) V dp + \left( \frac{c_v}{R} + 1 \right) p dV. \quad (7)$$

Considering the relations (8), (9) and (10) between the universal gas constant  $R$  and both the specific heats  $c_p$  and  $c_v$  at constant pressure and constant volume, respectively:

$$R = c_p - c_v \quad (8), \quad \gamma = \frac{c_p}{c_v} \quad (9), \quad \frac{c_v}{R} = \frac{1}{\gamma - 1} \quad (10),$$

the final equation for the net heat  $\delta Q_{net}$  over the crank angle increment  $d\theta$  can be derived as follows:

$$\frac{dQ_{net}}{d\theta} \cong \left( \frac{1}{\gamma - 1} \right) p \frac{dV}{d\theta} + \left( \frac{\gamma}{\gamma - 1} \right) V \frac{dp}{d\theta}, \quad (11)$$

where:

$\gamma$  - ratio of the specific heats ( $c_p/c_v$ ) at constant pressure and constant volume, respectively,

$p$  - in-cylinder combustion pressure,

$V$  - in-cylinder volume,

$\theta$  - crank angle (CA) deg,

$Q_{net}$  - net heat released during combustion.

The equation (11) is applied for heat release rate (HRR) determination in the IC engine [5,11,12,13,14].

In accordance with this equation, combustion progress can be expressed by the cumulative heat  $Q_{net}$ , which can be determined through integrating it over the  $\theta$ .

If someone assumes that the Lower Heating Value (LHV) of the fuel does not change at elevated pressure and temperature, then the heat released from combustion process can be expressed as a product of the fuel LHV and the fuel mass burnt  $M_f(\theta)$ . Thus, progress in combustion can be quantitatively described by the normalized function as the MFB (Mass of fuel Fraction Burnt) defined as follows:

$$MFB(\theta) = \frac{M_f(\theta)}{M_T} = \frac{Q_{net}(\theta)}{Q_{net}}, \quad (12)$$

where:

$M_f$  – mass of the fuel burnt since start of combustion up to the current crank angle  $\theta$ ,

$M_T$  – total mass of the fuel burnt in the single combustion event.

Although the MFB function is often used in the engine combustion analysis, difficulties as pointed in [15,16,17,18,19] might be encountered for anyone who wants to compute progress in combustion in the internal combustion (IC) engine on the basis of this equation (11). As far as both the  $p(\theta)$  and  $V(\theta)$  are known values, then the solution of the equation can be easily obtained. The problem appears in case when accurate determination of the  $\gamma$  ( $c_p/c_v$ ) ratio is required. There are several methods for calculating the  $\gamma$ . In general, these methods are based on empirical results. Gatowski et al. [20] proposed the  $\gamma$  can be determined as follows:

$$\gamma = 1.38 - 0.08 \cdot \frac{(T - 300)}{1000}, \quad (13)$$

where:

$T$  - temperature of the in-cylinder working fluid in K.

There are slightly different formulas for the  $\gamma$  determination in the [21] and [22].

$$\gamma = 1.338 - 6 \cdot 10^{-5} T + 10^{-8} T^2, \quad (14)$$

$$\gamma = 1.38 - k_1 e^{\left(\frac{k_2}{T}\right)}, \quad (15)$$

where:  $k_1$  and  $k_2$  are constants from the range (0.2 - 900).

As anyone can notice, these equations are also functions of temperature.

Furthermore, the  $\gamma$  can be determined directly, following its definition on the basis of separate calculation of the  $c_p$  and  $c_v$ . In this case both the  $c_p$  and  $c_v$  can be determined from e.g. the NASA polynomials. During combustion, relation between burnt and unburnt air-fuel mixture varies, that contributes to change in the  $\gamma$ . Thus, the  $\gamma$  is changing from the  $\gamma_u$  to the  $\gamma_b$  which stand for the unburnt and burnt mixture, respectively. To compute the final  $\gamma$  for the total burnt and unburnt compounds of the fluid filling the engine cylinder, the mass-based ratio between burnt and unburnt content have to be provided. As the combustion progress requires  $\gamma$  value for its computation, thus both combustion progress represented by the released heat and the  $\gamma$  can be determined from an iteration process. As mentioned, the total  $\gamma$  of burnt and unburnt species can be determined on the basis of their mass fractions. Therefore, the MFB profile for the combustion progress is required. The most well-known function for MFB calculation is the empirical formula developed by Rassweiler and Withrow [23]. It is presented in the equation (16).

$$MFB_{\theta} = \frac{\sum_{\theta} \Delta p_{\theta}}{\sum \Delta p_{begin-end}}, \quad (16)$$

where:

$\theta$  – crank angle,

$\Delta p_{\theta}$  – corrected pressure rise with respect to combustion,

*begin – end* – location of begin and end of combustion.

However, the difficulty has to be faced with the proper determination of the end of combustion, which is necessary for the MFB computation. Brunt et al. [24] assumed that the end of combustion is located at the maximum of  $pV^{1.15}$ .

## RESULTS AND DISCUSSION

The main aim of the paper is to show that the combustion progress in the IC engine can be expressed by the normalized cumulative net heat represented by the MFB function. In that case no one takes care about determining the  $\gamma$  with relatively high accuracy. Unlike the MFB, which is considered as pure empirical formula, the cumulative net heat is obtained through applying Energy Conservation Law for that purpose. Although normalized net heat cannot be managed as the MFB profile due to neglecting heat transfer to walls and the crevice effect, it can be applied as well as the empirical MFB formulas for the MFB determination. Furthermore, such approach is justified with respect to theory.

For example, combustion of hydrogen at stoichiometric ratio with exhaust gas recirculation (EGR) of 20% (by mass) was taken into analysis. The combustion pressure was acquired from the IC spark ignited CFR engine (displacement = 611cm<sup>3</sup>) working at compression ratio (CR) of 10 with spark timing (ST) of 6 deg before TDC at rotational speed of 900rpm. In Figure 1 the in-cylinder combustion pressure vs crank angle is plotted. As seen, there are pressure fluctuations on the combustion pressure as a result of hydrogen combustion instabilities.

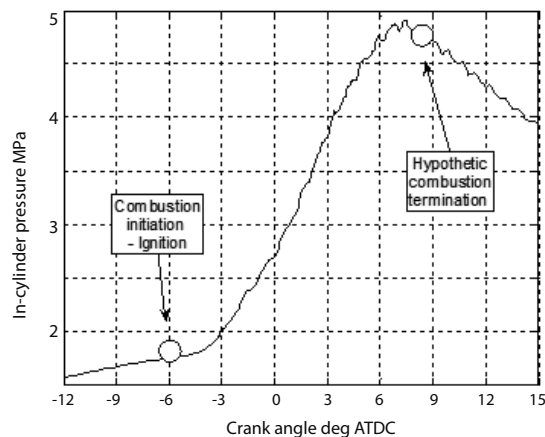


Fig. 1. In-cylinder combustion pressure history of hydrogen combustion at stoichiometric ratio with 20%EGR in the CFR engine with compression ratio of 10 and spark timing of 6 deg before TDC

As far as combustion progress is going on the chemical composition of the gases filling the combustion chamber is also varying from air and fuel (hydrogen and EGR gases) at the start of combustion to exhaust gases when combustion is completed. Hence, the  $\gamma = c_p/c_v$  ratio is also changing with the in-cylinder gas chemical composition change, as it is plotted in Figure 2.

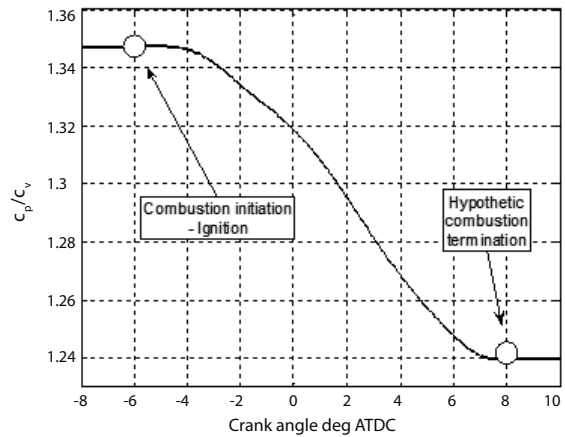


Fig. 2. Estimated  $\gamma$  ( $c_p/c_v$ ) of the in-cylinder gases during combustion of H<sub>2</sub>+air+20%EGR in the CFR engine (CR = 10, ST = -6 deg ATDC) vs crank angle

To show the impact of the  $\gamma$  on the heat release calculation and further, on the MFB function, four cases of various  $\gamma$  were taken for the analysis. They are shown in the table 1.

Table 1: Four cases of the  $\gamma$  taken for MFB calculation

No.	$\gamma = c_p/c_v$	@ temperature	Air-fuel mixture composition
1	1.396 (constant)	25°C (NTP)	Hydrogen+air <sub>stoic</sub> +20%EGR
2	1.347 (constant)	900K (temperature at the ignition)	Hydrogen+air <sub>stoic</sub> +20%EGR
3	Varied from 1.34 to 1.24	Varied from 900K to 2500K	Hydrogen+air <sub>stoic</sub> +20%EGR
4	$\gamma = n$ , Constant, assumed as polytropic index $n$ of compression	Unknown	Hydrogen+air <sub>stoic</sub> +20%EGR

In the case 4 the  $\gamma$  is assumed to be the polytropic index  $n$  of the compression process in the piston engine following the equation (17):

$$\gamma = \frac{\log \frac{p_0}{p_i}}{\log \frac{v_i}{v_0}}, \quad (17)$$

where:

$p_0, v_0$  - pressure and volume at spark timing, respectively,

$p_i, v_i$  - pressure and volume at point  $i$  located before the spark timing with  $p_0, v_0$ ,  
 $i - 1, 2, 3$  - index of the point  $i$  with  $p_i, v_i$  taken for  $\gamma$  computation (Fig. 3).

As shown in Figure 3 the compression process in the  $\log p - \log v$  coordinating system is represented by almost the straight line. As the in-cylinder pressure increases with the in-cylinder volume decrease, the average temperature of the in-cylinder gases also increases, which causes higher heat transfer rate to the engine cooling system, therefore the instantaneous polytropic index  $n$  decreases with compression process approaching the ignition point expressed by the  $p_0, v_0$  coordinates. Thus, someone can assume that the polytropic index  $n$  can be similar to the  $\gamma$  when it is calculated at the end of the compression stroke eg. assuming the data for  $p_0, v_0$ , and  $p_1, v_1$ .

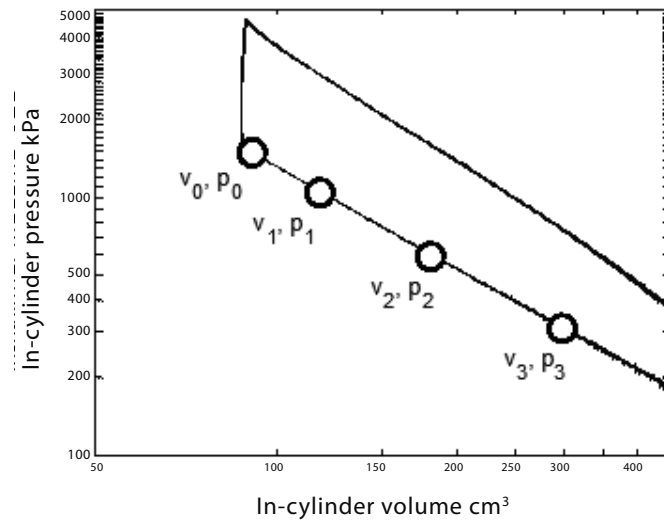


Fig. 3.  $p$ - $v$  diagram in log scale with points marked for polytropic index computation

Following the equation (11), the heat release rate (HRR) was calculated using the real combustion pressure. Due to differentiating the  $dp/d\theta$  expression, undesired influence of pressure fluctuations on the heat release appeared. To avoid this shortcoming, low-pass filtering the combustion pressure with the cut-off frequency of 3.5 kHz was applied. Then, the pressure fluctuations were eliminated from the combustion pressure trace. As a result, the computed HRR curve was smooth, as presented in Figure 4a, in which the HRR vs crank angle computed with 3 different  $\gamma$  ( $c_p/c_v$ ) values is presented. As expected, higher  $\gamma$  results in lower HRR. Another feature can also be observed Figure 4a. It was found that all the three curves were similar in shape to each other, even though they were computed with different  $\gamma$ 's. Furthermore, cumulative net heat profiles for these  $\gamma$  ratios (Figure 4b) also look similar to each other. The noticeable difference is in the maximum HRR and maximum cumulative heat, which is justified if anyone assumes that coefficients  $\gamma/(\gamma+1)$  and  $1/(\gamma+1)$  (Eq.11) can vary with  $\gamma$  change.

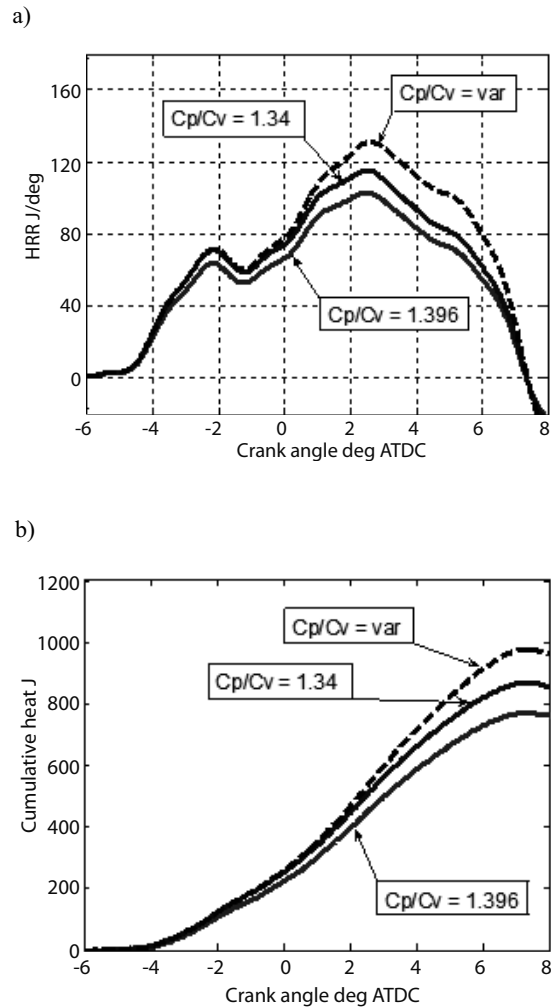


Fig. 4. HRR vs crank angle (a), cumulative net heat vs crank angle (b)

The difference in the cumulative heat between these curves presented in Figure 4b can be reduced if they are recalculated to normalized interval from 0 to 1, as shown in Figure 5a. Figure 5b depicts zoom onto 0.5 of the MFB. In the percentage scale this value corresponds to 50%MFB. There are limits in the MFB profile, which are particularly important in the analysis of the combustion process. They divide the combustion process into combustion phases as follows:

- 0-0.1MFB (0-10%MFB) – first combustion (or pre-combustion) phase,
- 0.1-0.9MFB (10-90%MFB) – main combustion phase – it is treated as combustion duration when expressed in CA deg.

0.5MFB (50%MFB) is treated as the centre of combustion. In its crankshaft location half of the fuel amount has been burnt.

The curve calculated for the  $\gamma$  varying with combustion progress (Table 1, case No.3) was considered as the most accurate to the real heat release, so it was taken as the reference trace to the others. As seen, the largest difference occurs for location of 0.5MFB (50%MFB) and it equals approximately to 0.16 CA deg. As far as the 0.1MFB and 0.9MFB are concerned, they are shifted to the same direction and the offset is almost the same. Thus, the combustion duration as measured from 0.1 to 0.9MFB might be charged with insignificant error when compared to the real 0.1-0.9MFB combustion phase.

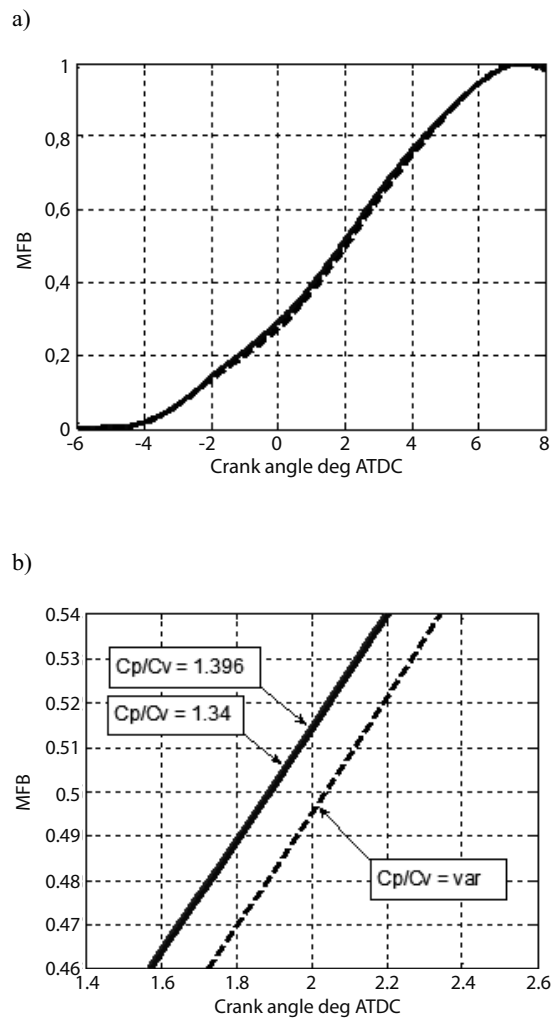


Fig. 5. MFB profile (a), zoom to 0.5MFB (b)

As mentioned, there are several difficulties in calculating the  $\gamma$  ( $c_p/c_v$  ratio), so, the polytropic index  $n$  of the compression stroke can be applied instead of the specific ratio  $\gamma$  as recommended by Tunestal [25]. As determined, the polytropic index  $n = 1.34$  of the combustion pressure trace



data taken at the end of the compression stroke does not vary remarkably when compared with the  $\gamma = 1.347$  for the combustible mixture. Satisfactorily good compatibility between  $\gamma$  and  $n$  in this case comes from low heat transfer between walls and the in-cylinder fluid at the end phase of the compression stroke.

## CONCLUSIONS

Progress in combustion determined as the normalized cumulative net heat on the basis of the Energy Conservation Law can be considered as good as the other methods for heat release rate (HRR) and MFB analysis in the IC engine. It provides several advantages such as satisfactory accuracy and simplified calculation, in which  $\gamma = c_p/c_v$  ratio can be calculated as the compression polytropic index directly determined from the compression pressure trace. Such assumption does not charge the final results with significant errors. Additionally, normalized net heat can be considered as substitution for the MFB, which usually is empirically determined. This approach for combustion progress analysis was successfully applied for combustion knock in the hydrogen fuelled IC engine [26].

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#### UPROSZCZONA METODA OBLICZANIA POSTĘPU SPALANIA W SILNIKU O SPALANIU WEWNĘTRZNYM

**Streszczenie.** W artykule przedstawiono uproszczoną metodę obliczania MFB (części spalanej masy) w oparciu o zasadę zachowania energii. Początkowo, ciepło skumulowane w funkcji kąta obrotu wału korbowego jest obliczane w wyniku rozwiązania powyższej zasady. Dalej, skumulowane ciepło po normalizacji może być

traktowane jako funkcja MFB. Ponadto, wyliczono też stosunek ciepła właściwego  $c_p/c_v$ , a uzyskane wyniki prowadzą do wniosku, że dokładność w określaniu  $c_p/c_v$  nie wpływa znacząco na kształt znormalizowanego profilu MFB. Ponadto, przy zastosowaniu przedstawionej metody obliczeniowej, fazy spalania 0-10% MFB i 10-90% MFB są obciążone marginalnym błędem.

**Słowa kluczowe:** silnik spalinowy, szybkość uwalniania ciepła, MFB (część spalona masy).