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ICE GROSS HEAT RELEASE STRONGLY INFLUENCED BY SPECIFIC HEAT RATIO VALUES

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ABSTRACT–Several models for the evaluation of Gross Heat Release from the internel combustion engine (ICE) are often used in literature. One of these is the First Law – Single Zone Model (FL–SZM), derived from the First Law of Thermodynamics. This model presents a twice advantage: first it describes with accuracy the physic of the phenomenon (charge heat release during the combustion stroke and heat exchange between gas and cylinder wall); second it has a great simplicity in the mathematical formulation. The evaluation of Heat Release with the FL–SZM is based on pressure experimental measurements inside the cylinder, and on the assumption of several parameters as the specific heat ratio, wall temperature, polytropic exponent for the motored cycle evaluation, and many others. In this paper the influence of gases thermodynamic properties on Gross Heat Release has been esteemed. In particular the influence of an appropriate equation for $k = k(T)$ (specific heat ratio vs. temperature) which describes the variations of gases thermodynamic properties with the mean temperature inside the cylinder has been evaluated. This equation has been calculated by new V order Logarithmic Polynomials (VoLP), fitting experimental gases properties through the least square methods.

KEY WORDS : ICE (International Combustion Engine), Heat release, Logarithmic polynomials

NOMENCLATURE

Q_{hr} = gross heat release
$k(T)$ = specific heats ratio variable with the mean gas temperature
T = charge mean temperature inside the cylinder
p = pressure measured inside the cylinder
V = volume swept from the piston
Q_w = heat exchanged with the cylinder wall
U_s = internal sensible energy
Q = Q_{hr}–Q_w
W = work due to the piston motion
m = trapped mass
$c_v(T)$ = specific heat at constant volume, variable with temperature
$c_p(T)$ = specific heat at constant pressure, variable with temperature
Nu = Nusselt number
Re = Reynolds number
b = Reynolds exponent in the thermal exchange correlation
B = bore
C_1 = calibration constant
C_2 = calibration constant
w = characteristic charge velocity
π_p = piston mean velocity
p_m = pressure of the motored cycle
p_0, V_0, T_0 = reference pressure, volume and temperature
Φ = equivalence ratio
$\bar{\rho}$ = compression ratio
m_b = burned mass
m_u = unburned mass
$k_b(T)$ = specific heat ratio for the burned mass
$k_u(T)$ = specific heat ratio for the unburned mass
ϑ = crank angle
ϑ_0 = start of combustion crank angle
$\Delta\vartheta$ = total combustion duration
a, m = Wiebe function parameters
T_{SOI} = start of ignition temperature
T_{max} = highest temperature in the combustion chamber
c_{pu} = specific heat at constant pressure for the unburned mass
c_{pb} = specific heat at constant pressure for the burned mass
R_u, R_b = unburned and burned gas constant

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1. INTRODUCTION

Pressure measurements in thermodynamics analysis are a very powerful tool for the determination of the parameters that characterized ICE combustion. The principal approaches are the calculation of Mass Fraction Burned (MFB) for the determination of the characteristic crank angles in the combustion stroke, and the Heat Release analysis. Heat Release analysis brings to the determination of the Rate Of Heat Release (ROHR), a useful tool for the evaluation of combustion noise and NO_x emissions, and to Cumulative Heat Release utilized for the determination of the principal combustion characteristics, as the combustion efficiency.

Due to the great importance of Heat Release analysis, several models have been developed in the last years. One of first simple models (Rassweiler and Withrow, 1938) needs only pressure data but presents a great disadvantage: the assumption of a constant value for the polytropic exponent, when really it is well known that different values occur for the compression and expansion strokes, and during the combustion phase.

Several models were elaborated, from the most simple (McCuiston *et al.*, 1977), in which the results are affected from an error due to the assumption to neglect volume variation during the combustion stroke, to the most complex bi– or three-dimensional models (Kamimoto *et al.*, 1977; Sastry and Chandra, 1994) which present the same results of the best 1-D models and a major mathematical complexity and computational weight.

A Single Zone Model, simple and accurate, was developed by Gatowski et al. (Gatwoski *et al.*, 1984), and after optimized (Chun and Heywood, 1993) for a charge with high swirl motion.

The present model is based on the First Law of Thermodynamics (First Law Model) and usually it is utilized in four different forms: 1) Basic First Law (k = cost. and absence of heat exchange between gas and cylinder wall); 2) First Law and Heat Transfer (k = cost. and heat exchange between gas and cylinder wall); 3) First Law with Variable Specific Heats ($k = k(T)$ and absence of heat exchange between gas and cylinder wall); 4) First Law with Variable Specific Heats and Heat Transfer ($k = k(T)$ and heat exchange between gas and cylinder wall).

Often in literature, when First Law Model is used, a constant value for k is chosen. Only with a great experience in this research area it is possible to choose the exact value for k that brings to the same results of an analysis based on gas specific heats ratio variable with the temperature.

The sub-model 4) is the model that furnishes the most reliable results (Brunt *et al.*, 1997).

2. FIRST LAW WITH VARIABLE SPECIFIC HEATS RATIO AND HEAT TRANSFER

The equation for the evaluation of the heat release can be inferred from (Gatwoski *et al.*, 1984; Brunt and Platts 1999) and is:

$$dQ_{hr} = \frac{k(T)}{k(T)-1} p dV + \frac{1}{k(T)-1} V dp + dQ_w \tag{1}$$

Equation (1) is obtained from the first law of thermodynamics, for closed systems:

$$dU_s = dQ + dW \tag{2}$$

with

$$\begin{aligned} dW &= -p\ dV \\ dU_s &= m\ c_v(T)\ dT \\ dT &= d(pV)/mR \\ R/c_v(T) &= k(T)-1 \end{aligned} \tag{3}$$

(with the assumption that the gas constant R does not change during the combustion process).

Substituting Equation (3) in (2) and rearranging the terms, it is possible to obtain the traditional equation (1) for Heat Release.

In this research, to model the heat exchange between gas and cylinder wall, has been utilized the Woschni model (Woschni, 1967). In this model, applied to ICE, the heat exchange coefficient is:

$$h_c = 3.26 C_1 B^{b-1} p_b T^{0.75-1.62b} w^b \quad [\mathrm{W/(m^2K)}] \tag{4}$$

In equation (4) b is set to 0.8 (from thermal exchange correlation: $Nu = C\ Re^{0.8}$); B is expressed in [m], p in [kPa] and T in [K]; the characteristic charge velocity, due to piston motion and to combustion process, is expressed in [m/s]:

$$w = 2.28 \bar{u}_p + 3.24 \times 10^{-3} C_2 \frac{V T_0}{p_0 V_0} (p - p_m) \tag{5}$$

p_0, V_0, T_0 can be referred at IVC or at SOI.
For the evaluation of p_m a polytropic equation as

$$p_m = p_0 \left(\frac{V_0}{V} \right)^n \tag{6}$$

was utilized (Chun and Heywood, 1993), where n is usually set to 1.3, since variation from 1.25 and 1.35 has no significant effect on the heat exchange between gas and cylinder wall, and neither on the Gross Heat Release.

In this application, variation from 1.25 and 1.35 brings to a maximal error of ±0.4% on the Q_w, and to an error of ±0.1% on the Gross Heat Release.

In the heat transfer model, the constants C_1 and C_2 was included to allow the model to be adjusted easily. These two constants are not physical quantities and may differ from engine to engine (Chun and Heywood, 1993). Therefore these two constants are calibrated with actual engine data.

2.1. Specific Heat Ratio Influence on Gross Heat Release

Several parameters are present inside the mathematical model for the Gross Heat Release evaluation. Since the specific heat ratio k has a great influence on the heat release peak and on the shape of the heat release curve (Brunt *et al.*, 1998), many researchers have elaborated different mathematical equations to describe the dependence of k from temperature. First and second order equations have been elaborated: $k(T) = a + bT$ (Heywood, 1988) and $k(T) = a + bT + cT^2$ (Brunt *et al.*, 1998).

Starting from this assumption, the objective of this paper is to develop and to implement a First Law – Single Zone modified model for the heat release inside ICE, where k is temperature dependent, with a VoLP functional form:

$$k(T) = f\{a_0 + a_1 \ln(T) + a_2 [\ln(T)]^2 + \ldots + a_5 [\ln(T)]^5\}$$

To verify the model accuracy, it has been implemented for the calculation of the Gross Heat Release for a CFR engine, fuelled with 2,2,4-Trimethylpentane, engine speed = 600 r/min, $\Phi = 1$, $\bar{\rho} = 5.8$.

In Figure 1 it is shown the great influence of k value on the Cumulative Gross Heat Release, while in Figure 2 it is possible to see how k has not a meaningful influence on the MFB. For a correct evaluation of the heat release it is necessary to use a mathematical function, which describes with accuracy the trend of k with the temperature.

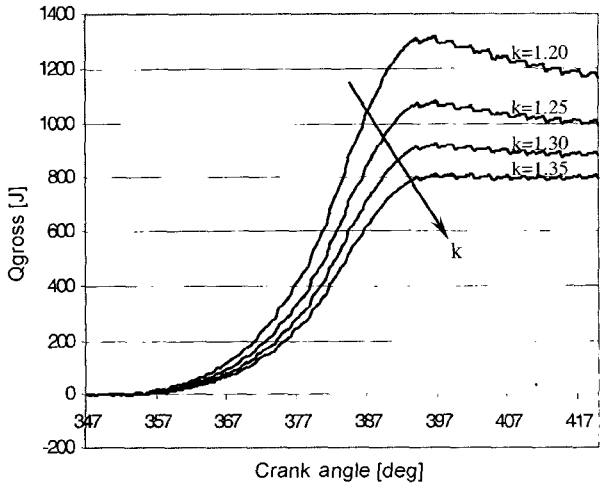

Figure 1. Cumulative gross heat release trend at various k (SOI at 347° - TDC at 360°).

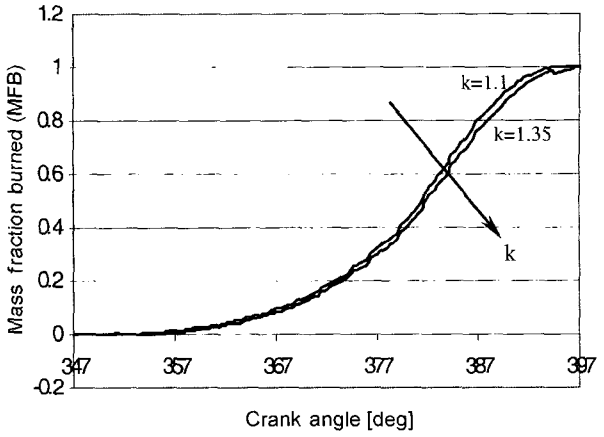

Figure 2. MFB dependence from k.

2.2. Determination of Specific Heats Ratio $k = k(T)$

2.2.1. Mass fraction burned

Since k is depending on temperature and on charge composition, and since MFB is not depending on the value chosen for the constant k (see Figure 2), it is possible to write for the function $k(T)$:

$$k(T) = k_b(T)x_b(T) + [1 - x_b(T)]k_u(T) \tag{7}$$

and $x_b(T)$ can be evaluated from the Cumulative Gross Heat Release with $k = \text{cost.}$ starting from:

$$x_b(\vartheta) = \frac{m_b}{m_u + m_b} = \frac{Q_{gross}|_{\max}}{Q_{gross}(\vartheta)} \tag{8}$$

where:

$$Q_{gross}(\vartheta) = \sum_{SOI}^{\vartheta} \Delta Q_{hr} \tag{9}$$

Evaluated $x_b(\vartheta)$ (Figure 3) and the "T – ϑ" relationship (Figure 5), it is possible to evaluate the trend of x_b with the mean charge temperature (Figure 4), and so implement $x_b(T)$ inside Equation (7).

Figure 3 represents the comparison between the MFB (evaluated through the experimental pressure measurements and applying the First Law – Single Zone Model (1) with $k = 1.3$), the Wiebe Equation and sixth order traditional polynomial interpolation using the least square method.

The Wiebe function is:

$$x_b(\vartheta) = 1 - \exp\left[-a\left(\frac{\vartheta - \vartheta_0}{\Delta\vartheta}\right)^{m+1}\right] \tag{10}$$

The parameters a and m have been chosen to maximize the correlation factor R^2: a and m are adjustable parameters (Heywood, 1988).

In this application the fitting polynomial (Poli. Experi-

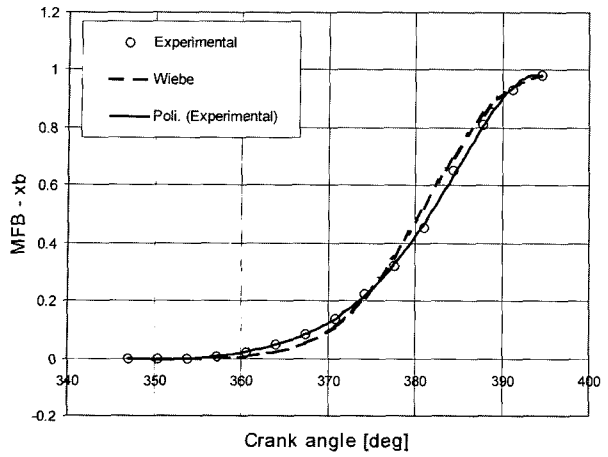

Figure 3. Mass fraction burned *vs.* crank angle.

Table 1. MFB crank angle errors.

	x_b=0.1	x_b=0.5	x_b=0.9
Wiebe	1.9°	1.1°	0.5°
VI order Poli.	0°	0.3°	0.2°

mental in Figure 3) is represented by: $x_b(\vartheta) = a_0 + a_1\vartheta + a_2\vartheta^2 + \cdots + a_6\vartheta^6$.

Table 1 shows the crank angle error referred to the Wiebe function and to the VI order polynomial, when x_b=0.1, x_b=0.5, x_b=0.9.

Figure 4 represents the MFB trend with mean charge temperature. Experimental data on x_b and other three curves are represented: 1) Log. Pol., 2) Linear Interpol., 3) Axis without Interp. These three curves fit experimental data respectively with a VoLP, with a linear interpolation, and with an axis passing through the first and the last experimental points (Equation 11). All three curves present a high correlation factor R^2, so that it is possible to choose the curve with the simplest mathematical functional form (Equation 11).

The equation for the axis passing through the first and the last experimental points (R^2=0.997) is:

$$\begin{aligned} x_b(T) &= 0 && \text{for } T < T_{SOI} \\ x_b(T) &= \frac{T - T_{SOI}}{T_{max} - T_{SOI}} && \text{for } T_{SOI} \le T \le T_{max} \\ x_b(T) &= 1 && \text{for } T > T_{max} \end{aligned} \qquad (11)$$

Figure 5 reports the temperature and MFB experimental trends with crank angle. It is possible to notice as the maximum value of the MFB correspond to the maximum value of temperature, while the MFB start to be different from zero, only after the Start Of Ignition (SOI = 347° crank angle).

2.2.2. Burning and unburning specific heat ratio

The function $k = k(T)$ is the ratio of specific heat at constant pressure $c_p(T)$, and specific heat at constant volume $c_v(T)$. So, an accurate function for $k(T)$ is depending on an accurate evaluation of $c_p(T)$.

The function adopted to fit experimental data on c_p gases, is a VoLP (Equation 12). This choice is derived from precedent researches of the authors (Lanzafame and Messina, 2000; Lanzafame and Messina, 2001a; Lanzafame and Messina, 2001b; Lanzafame and Messina, 2002) in which several VoLP advantages have been showed: 1) high fitting accuracy (R^2 > 0.99); 2) the capacity to fit experimental data on large temperature ranges only with a single VoLP; 3) possibility to extrapolate experimental data beyond experimental

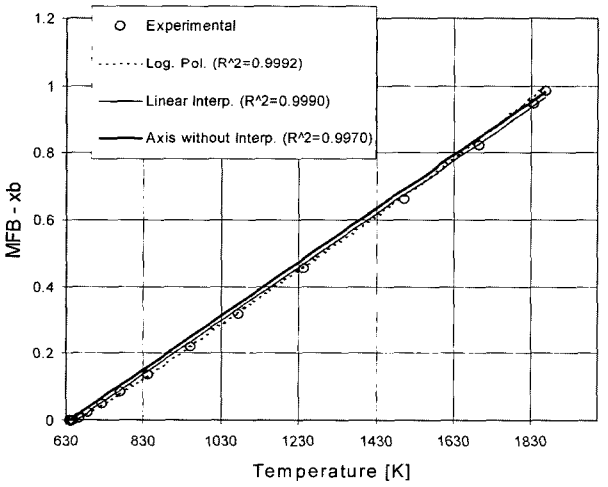

Figure 4. Mass fraction burned *vs.* temperature.

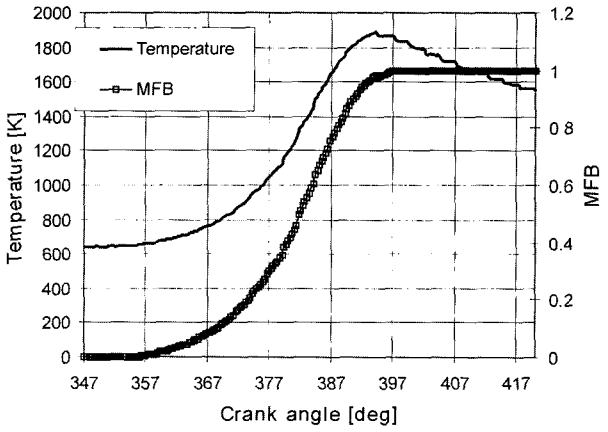

Figure 5. Temperature and x_b trends *vs.* crank angle.

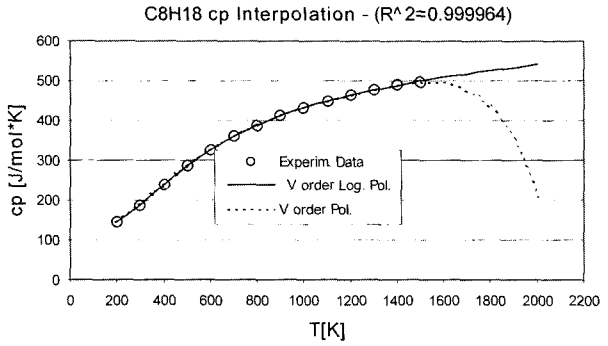

Figure 6. Comparison between traditional interpolation and new Logarithmic Polynomial interpolation.

temperature range.

The functional form of a VoLP for the c_p is:

$$c_p(T) = a_0+a_1\ln(T)+a_2[\ln(T)]^2 +a_3[\ln(T)]^3+\ldots+a_5[\ln(T)]^5 \quad (12)$$

where a_0, .., a_5 are the constants to be evaluate through the least square method (Milton and Arnold, 1986), on the basis of c_p experimental data. Due to their high interpolation accuracy, VoLP can be utilized to extrapolate experimental data beyond experimental temperature range (see Figure 6) (Lanzafame and Messina, 2002).

In Figure 6, c_p experimental data on C_8H_{18} (Scott, 1974) have been fitted with a VoLP, and with a traditional V order polynomial ($c_p(T) = a_0 + a_1T + a_2T^2 + a_3T^3 +\cdots+ a_5T_5$). In the same figure we can see how the traditional polynomial cannot be used beyond experimental temperature, while a VoLP can be extrapolated for a 30%, with an error less than 1% (Lanzafame and Messina, 2002). Figure 6 is referred to the C_8H_{18}, but the same trend has been demonstrated for many other gases (Lanzafame and Messina, 2002).

In order to evaluate $c_p(T)$, a complete reaction of combustion has been considered, where the reagents of the reaction are fuel and technical air (21%$_v$ O_2 and 79%$_v$ N_2), while the products are constituted only by the species with a significant moles number (Sastry and Chandra, 1994; Heywood, 1988). The products considered are CO_2, H_2O and N_2. Fuel c_p experimental data have been taken from literature (Scott, 1974), and utilizing the least square method, the six constant a_0,..., a_5 have been evaluated (Table 2). In Table 2 are present also the VoLP coefficients for the other gases, and the relative temperature range of validity. Experimental data for all the other gases have been taken from JANAF Thermochemical Tables (JANAF, 1971).

Evaluated the c_p for each gas, c_{pu} and c_{pb} have been calculated:

$$c_{p_u}(T) = \frac{m_{C_8H_{18}}}{(m_{tot})_u}c_{p_{C_8H_{18}}}(T)+\frac{m_{O_2}}{(m_{tot})_u}c_{p_{O_2}}(T)+\frac{m_{N_2}}{(m_{tot})_u}c_{p_{N_2}}(T) \quad (13)$$

$$c_{p_b}(T) = \frac{m_{CO_2}}{(m_{tot})_b}c_{p_{CO_2}}(T)+\frac{m_{H_2O}}{(m_{tot})_b}c_{p_{H_2O}}(T)+\frac{m_{N_2}}{(m_{tot})_b}c_{p_{N_2}}(T) \quad (14)$$

and at the end $k_u(T)$ and $k_b(T)$ have been evaluated:

$$k_u(T)=\frac{c_{p_u}(T)}{c_{p_u}(T)-R_u} \quad (15)$$

$$k_b(T)=\frac{c_{p_b}(T)}{c_{p_b}(T)-R_b} \quad (16)$$

The Figures 7 and 8 show the k function, respectively depending on crank angle and temperature.

In Figure 7, when $x_b = 0$ the value of k (for the actual charge) is the same of the k for the unburned mass, while

Table 2. c_p VoLP coefficients [c_p]=[J/(mol K)].

Species	a_0	a_1	a_2	a_3	a_4	a_5	R^2
C_8H_{18} 200 < T < 2000 K	−43029.69896	36241.19904	−12036.09466	1966.430702	−157.61132	4.9695987	0.999964
O_2 273 < T < 3500 K	10228.342599	−7184.923331	2010.868084	−279.694958	19.348226	−0.532569	0.999662
N_2 273 < T < 3500 K	−7513.364197	5708.380466	−1712.173896	254.295542	−18.699837	0.544972	0.999927
CO_2 273 < T < 3500 K	−1412.367846	1288.467702	−452.811975	77.548094	−6.435215	0.207544	0.999993
H_2O 273 < T < 3500 K	−11780.764955	8490.521798	−2414.775747	339.336617	−23.542768	0.645407	0.999893

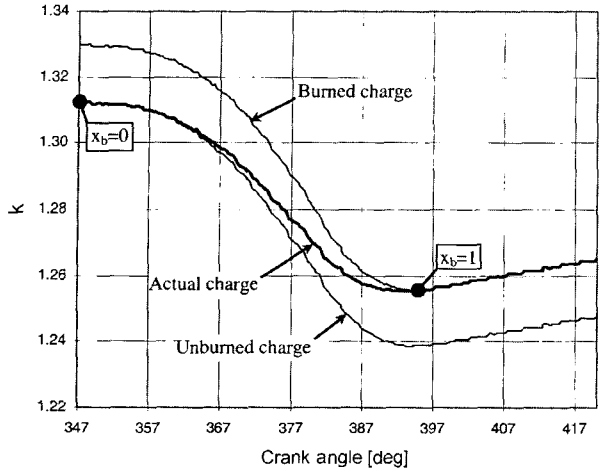

Figure 7. Variation of specific heat ratio with crank angle.

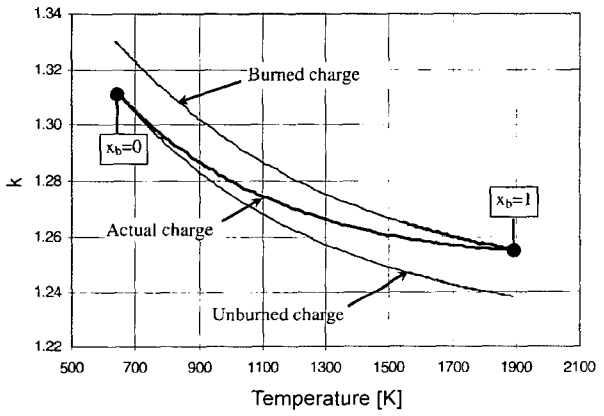

Figure 8. Variation of specific heat ratio with temperature.

in the case of $x_b = 1$ the k value for the actual charge is the same of that for the burned mass. For the crank angle between $x_b = 0$ and $x_b = 1$ k varies gradually, from the values of the unburned mass to the values of the burned mass. In Figure 8, k value depends on temperature. When temperature reach its peak value $x_b = 1$, after the temperature decrease, the mass is completely burned, and the k value for the actual mass is the same one of k for the burned mass.

2.2.3. Comparison with other $k(T)$ functions

Figure 9 shows a comparison between several k functions utilized in literature.

In Figure 9 the functions "k" and "k + gas res." represent the k functions utilized in this research: the first do not consider any fraction of residual gas in the cylinder, while the second considers a 10% of residual gas. The difference is very small, and the results on the heat release are the same. Residual gas fraction presents in the

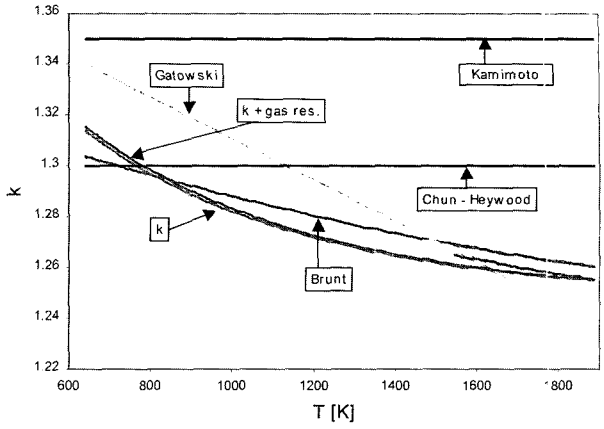

Figure 9. Comparison between several k functions utilized in literature.

cylinder creates a variation of the k function of about 0.1%, and a variation of 0.002% on the heat release calculated.

In Figure 9 are also represented several $k = k(T)$ functions (Brunt *et al.*, 1998; Chun and Heywood, 1987; Gatowsky *et al.*, 1984; Kamimoto *et al.*, 1977).

Brunt utilized a second order function, evaluated for a SI Engine, fuelled with C_8H_{16}. This function has been evaluated through a multi dimensional model, and it is the mean function among the k functions evaluated for $0.8 < \Phi < 1.2$. Gatowsky utilized an empirical formulas, implemented on a SI Engine, fuelled with C_8H_9N, and $\Phi = 1$. Kamimoto constant function (referred in (Kamimoto *et al.*, 1977) as model 1a) is utilized for a Diesel DI and it is evaluated through a comparison between a Single Zone Model and a Bi-Zone Model, in order to equalize the value of the heat release calculated. The same for the Chun and Heywood function, evaluated for a SI Engine. In all the models considered, the functions $k = k(T)$ have been evaluated for a specific application and derived from complex numerical models, or from the experience, or from single-zone and bi-zone models comparisons.

The authors suggest an alternative, simple and direct method for the calculation of the $k = k(T)$ function. The method is valid for any application and it needs only of gas thermodynamics properties, easily findable in literature, and of MFB, directly valuable from experimental pressure measurements.

2.3. Gross Heat Release Evaluation

Evaluated the effective correlation between k and T (and so between k and ϑ, since the correlation between T and ϑ derived from experimental measurements), the Gross Heat Release has been evaluated and compared with the Gross Heat Release calculated for k = cost. (see Figure 10 and 11).

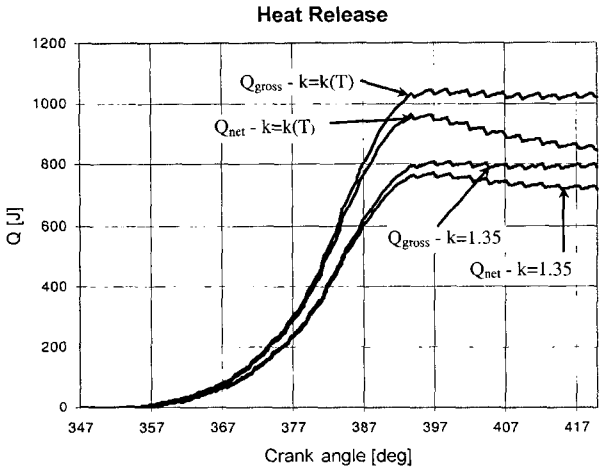

Figure 10. Comparison between four models for the Heat Release.

In Figure 10 is shown the comparison between four different models: 1) Q_{net} and k = cost: Heat Release without heat exchange between gas and wall cylinder and specific heat ratio constant; 2) Q_{net} and $k = k(T)$: Heat Release without heat exchange between gas and wall cylinder and specific heat ratio variable with the temperature; 3) Q_{gross} and k = cost: Heat Release with heat exchange between gas and wall cylinder and specific heat ratio constant; 4) Q_{gross} and $k = k(T)$: Heat Release with heat exchange between gas and wall cylinder and specific heat ratio variable with the temperature.

To evaluate Q_{gross} with k = 1.35, in the Woschni model the constants C_1 (Equation 4) and C_2 (Equation 5) have been set to 1. For the evaluation of Q_{gross} with $k = k(T)$, in the Woschni model the constant C_1 has been set to 1.69 and C_2 to 2.47.

The implementation of the Woschni model leads to an increment of the heat release peak of about 5% in the models with k = 1.35, and at an increment of 8.7% in the models with $k = k(T)$.

It is also important to underline as the difference between the last two models (Q_{gross} and k = cost and Q_{gross} and $k = k(T)$) is of 30%, while the choice of a $k = k(T)$ it is not important for the determination of the EEOC (Estimate End Of Combustion) crank angle. The difference between the last two models is due only at the value of the constant assigned at k in the model 3.

Varying the constant value of k in model 3, it is possible to find the value that cancels the difference between models 3 and 4 (see Figure 11). But the "a priori" exact choice of the constant to be assigned at k in the models 1 and 3, depends on different parameters, and it is difficult to put into practice the exact choice.

The implementation of a $k = k(T)$ function reduce notably the error deriving from a wrong choice of the constant for k.

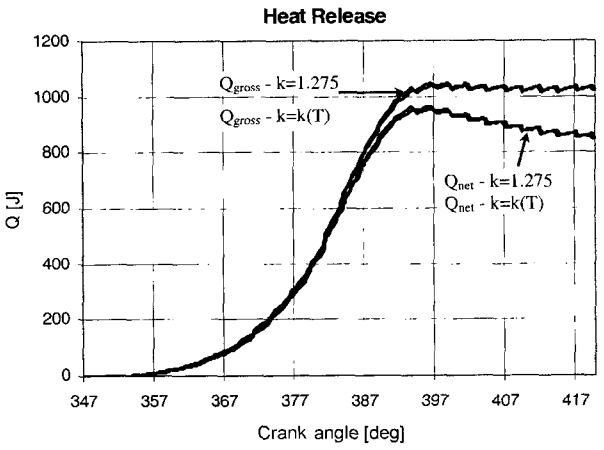

Figure 11. Exact choice for the constant k.

In this application the traditional single zone model coincide with the model proposed by the author only for k = 1.275. Changing engine, fuel or application, the exact value to be assigned at k will be varied, and only with a great experience it will be po

ssible to choose the correct value for k. Utilizing a $k = k(T)$ function it is possible to avoid this typology of error.

To verify the independence of x_b from the $k(T)$ function or from the constant value, Figure 12 shows the comparison between the MFB calculated with the four models. It is possible to notice the good accordance of the four MFB. In Figure 13 it is shown the comparison between the four models in the calculation of the Rate of Heat Release. Also in this case the value for the constant k is fundamental. The difference between the models with k = cost. and the

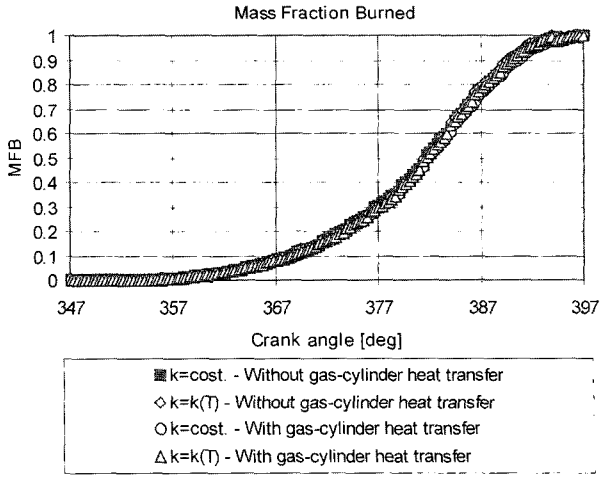

Figure 12. MFB for the four models.

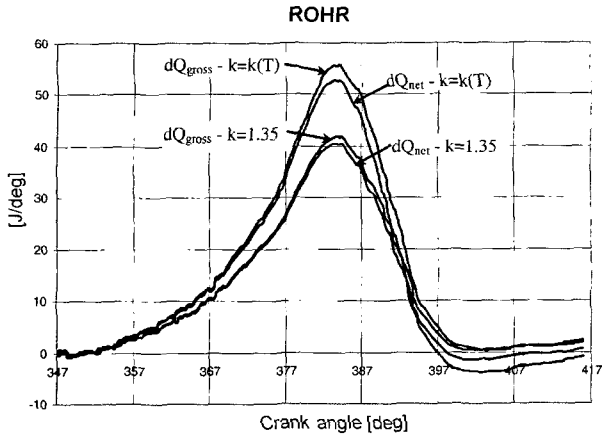

Figure 13. ROHR for the four models.

models with $k = k(T)$ is about of 30%, while do not have a great relevance the implementation of the Woschni model. The model influences only the final part of the RORH. The crank angle at which corresponds the RORH peak is the same in the four models.

3. CONCLUSIONS

In this research the influence of a specific heat ratio depending on temperature for the calculation of the Gross Heat Release inside ICE has been evaluated. For the evaluation of Gross Heat Release, the traditional First Law - Single Zone Model, modified by the authors, has been implemented. In this new model an original $k = k(T)$ function has been evaluated. This function has been obtained using new V order Logarithmic Polynomial (VoLP) to fit gases thermodynamic properties. Woschni model has been implemented for the heat exchange between gas and cylinder wall.

The implementation of a $k = k(T)$ function, instead of a constant value, do not affect the determination of combustion crank angles, but it is fundamental for the evaluation of the Gross Heat Release and of the Rate of Heat Release.

Very often in literature the First Law - Single Zone Model with a constant value for the specific heat ratio is utilized. The exact value for k depend on several parameters, which characterize the particular application, and only with a great experience it is possible to choice "a priori" the correct value for the constant k. An incorrect choice could bring to great errors, while the use of a correct function for $k = k(T)$ will bring with simplicity to the exact evaluation of the Gross Heat Release and of the Rate of Heat Release.

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