

## THERMODYNAMIC PROPERTIES OF WORKING FLUID OF INTERNAL COMBUSTION ENGINE

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### **Abstract**

*The objective of this study is to find a model of specific heat ratio taking into account the most significant features of engine working fluid.*

*Keywords: internal combustion engine, thermodynamic properties, heat release analysis.*

### **1. Introduction**

The understanding of the thermodynamic processes taking part in internal combustion engine is the key to engine optimisation which may be based on cylinder pressure feedback control. In-cylinder pressure changes are the crucial parameters affecting performance, thermal efficiency and emission of spark-ignition engine. Actually, the wide applications of pressure based techniques are limited due to high cost of the pressure sensor and the intrusive character of their application but it is expected that these difficulties will be overrun. Engine diagnostic methods based on the in-cylinder pressure signal may be also used for real-time calculations of the heat release ratio (HRR) and mass fraction burned (MFB). Quantitative analysis of these parameters may be useful for closed-loop control of IC engines.

Heat release analysis is important tool when developing IC engine and effective specific heat ratio model is necessary for such an analysis. The HRR calculations require some assumptions concerning the varying working medium composition. The following species can be identified as characteristic for the instantaneous cylinder charge composition:

- fresh mixture of the air and gaseous fuel (air-fuel-residuals mixture);
- products of combustion.

### **2. In-cylinder gas model**

The pressure  $p$ , specific volume  $v$  and temperature  $T$  relationship for gases is given by:

$$Z = \frac{pv}{RT} \quad (R \text{ denotes gas constant}) \quad (1)$$

Considerations of the generalized compressibility data can be concluded that the value of compressibility factor  $Z$  is approximately unity when the density of the gas is less than 1 mol/liter [5]. For high temperature,  $Z$  is closely equal to unity. Hence, the pressure, specific volume and temperature relation can be approximated by:

$$Z = \frac{pv}{RT} = 1 \quad \text{or:} \quad pv = RT \quad (2)$$

Equation (2) is referred to as ideal gas equation of state (EOS). For any gas, whose EOS is given exactly by equation (2), the specific internal energy depends on gas temperature only. This conclusion can be proved both formally [5] and experimentally [1].

The specification that constitute the ideal gas model are as follows:

$$pv = RT$$

$$u = u(T)$$

$$n = u(T) + pv = u(T) = RT = n(T)$$

The ideal gas model ignores the finite size of the molecules and the inter molecular forces. Consequently, as the gas becomes denser, the ideal gas EOS does not predict the relation between  $p$ - $T$ - $v$  with satisfactory accuracy (deviations are largest near the condensation point of the gas). If the molecular size and forces are included in the EOS of a gas, one refers to it as a real gas EOS. There are many (ca.100) equations of state that take molecular size and forces into account. The most popular of them (complexity, and accuracy considered) are van der Waals and Redlich-Kwong equations.

To verify the hypothesis that a gas (being the working fluid of internal combustion engine) can be modelled as an ideal gas, the thermodynamic states of interest were estimated for average spark-ignition and compression ignition engine. It can be seen (from the results presented in Fig. 1) that maximum value of the  $p/T$  quotient (characterizing the in-cylinder medium density) is about 2000 Pa/K for spark ignition engine and 12000 Pa/K for compression ignition engine. The compressibility factor  $Z$  was calculated using van der Waals and Redlich-Kwong EOS [1] over a range thermodynamic states [6,8]. The results, illustrated in Fig. 2, indicate that for SI engine the compressibility factor differs from that of an ideal gas by less than 1%.

For CI engine, the compressibility may have greater influence – at 12000Pa/K compressibility factor reaches up to 5%. Hence, an analysis of diesel cycle using ideal gas EOS overestimates the temperature. Implications of this can influence both exhaust gas chemistry and results of heat release rate calculations.

For the thermodynamic analysis of SI engine cycle, the ideal gas assumptions are fairly acceptable.

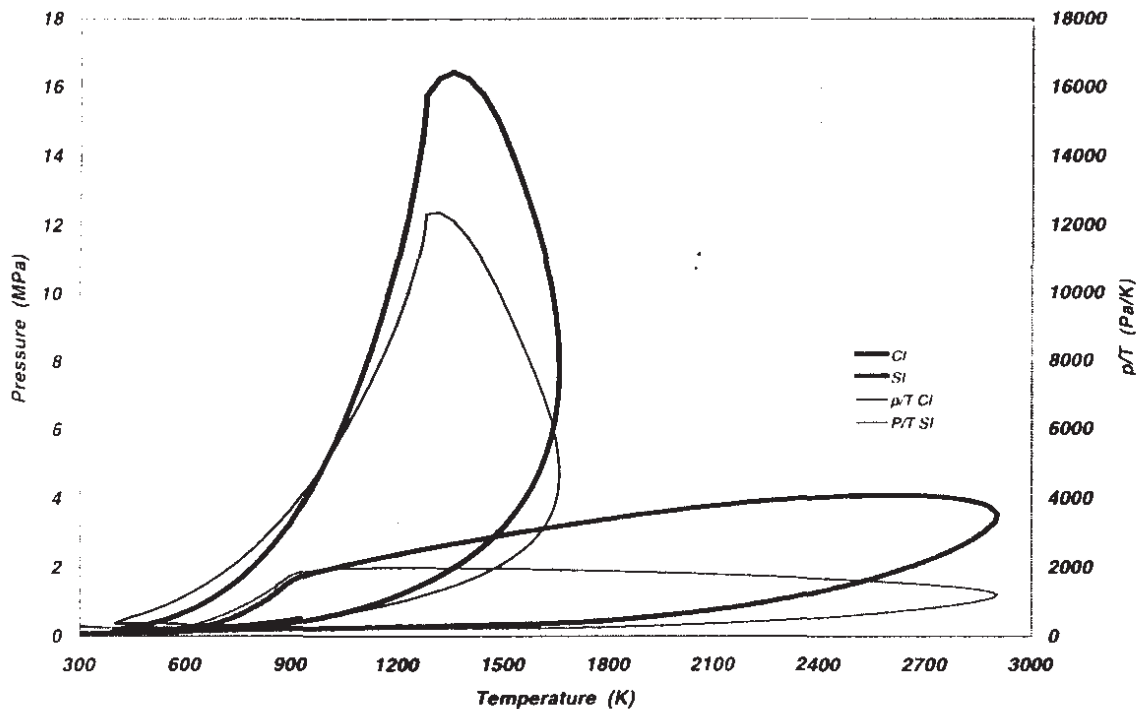


Fig. 1. Pressure and temperature ranges for SI and CI engine

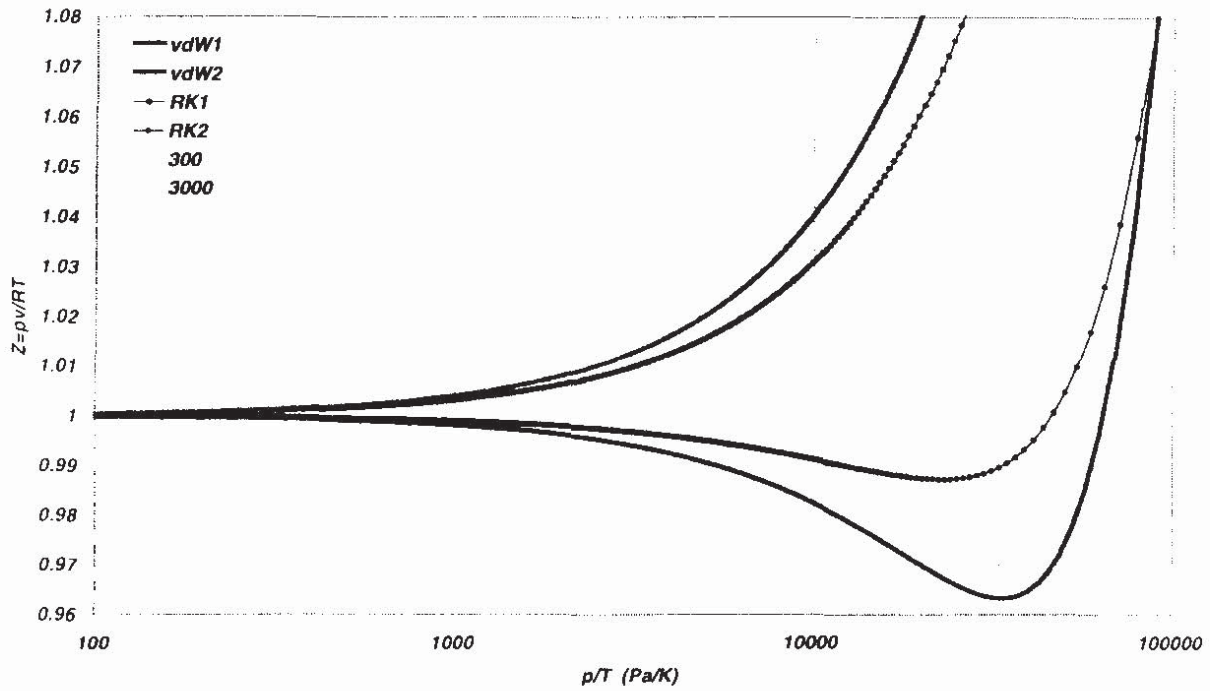


Fig. 2. Compressibility factors according to van der Waals and Redlich-Kwong EOS

### 3. Internal energy and specific heats of ideal gas.

For a gas obeying the ideal gas model specific internal energy depends only on temperature. Thus, the specific heat at constant volume defined by:

$$C_v = \left( \frac{\partial u}{\partial T} \right)_v \quad (3)$$

is also a function of temperature and hence

$$du = C_v(T) dT \quad (4)$$

Similarly, the specific enthalpy of ideal gas depends also on temperature only:

$$dh = C_p(T) dT \quad (5)$$

where  $C_p$  is defined by

$$C_p = \left( \frac{\partial h}{\partial T} \right)_p$$

For an ideal gas the specific heat ratio (important for engine heat release analysis):

$$\kappa = \frac{C_p(T)}{C_v(T)} = \kappa(T) \quad (6)$$

is also a function of temperature only.

Specific heat data are available in various form including graphs, tables and equations. For engine calculations, the most useful form is the polynomial one:

$$\frac{C_p}{R} = C_0 + C_1 T + C_2 T^2 + C_3 T^3 + C_4 T^4 \quad (7)$$

The values of the constants are listed in many sources (e.g. [10]) for several gases in the temperature range 300-3000 K (Fig. 4).

### 4. Specific heat ratio of the IC engine working fluid

The analysis of heat release rate in IC engine requires the knowledge of the ratio of specific heats for the involved working medium. The characteristics of that medium depends

mainly on engine combustion product composition which, in turn, depends on engine fuel, mixture composition and chemistry taken into account.

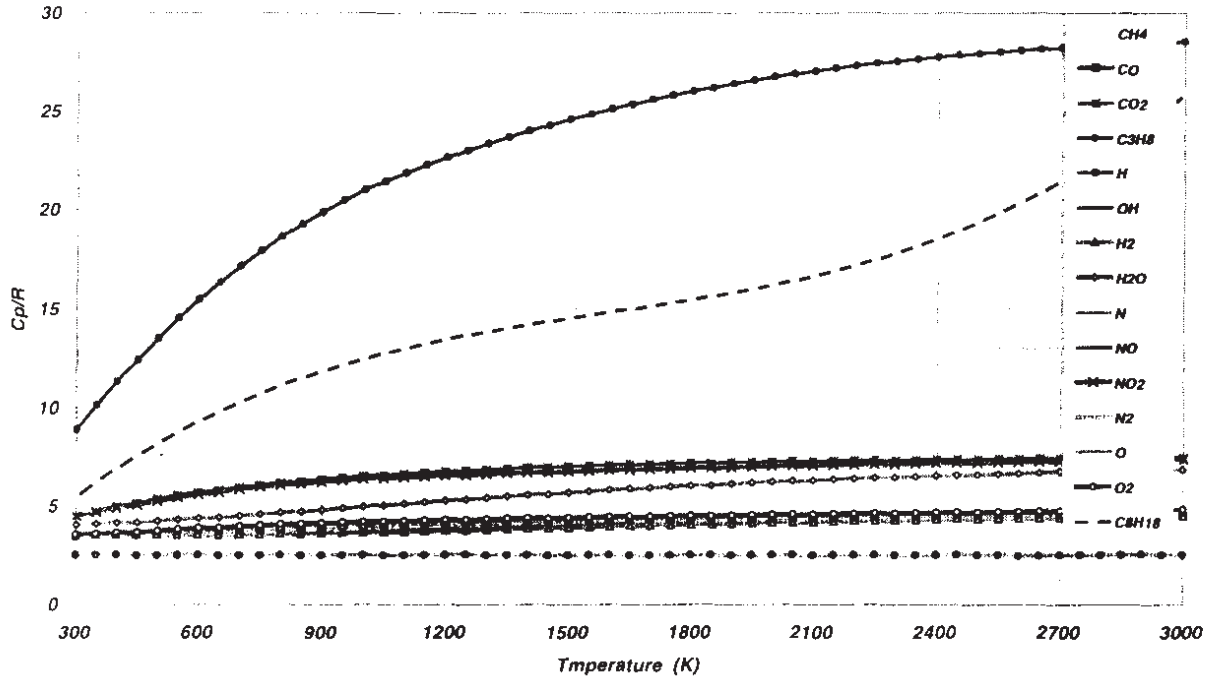
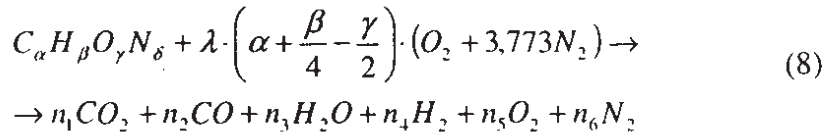


Fig. 3. Specific heat of engine working fluid components

At low temperature ( $T < 1000\text{K}$ , [2]) the overall combustion reaction for any air excess ratio  $\lambda$  can be written:



This equation assumes that the dissociation of the products is negligible.

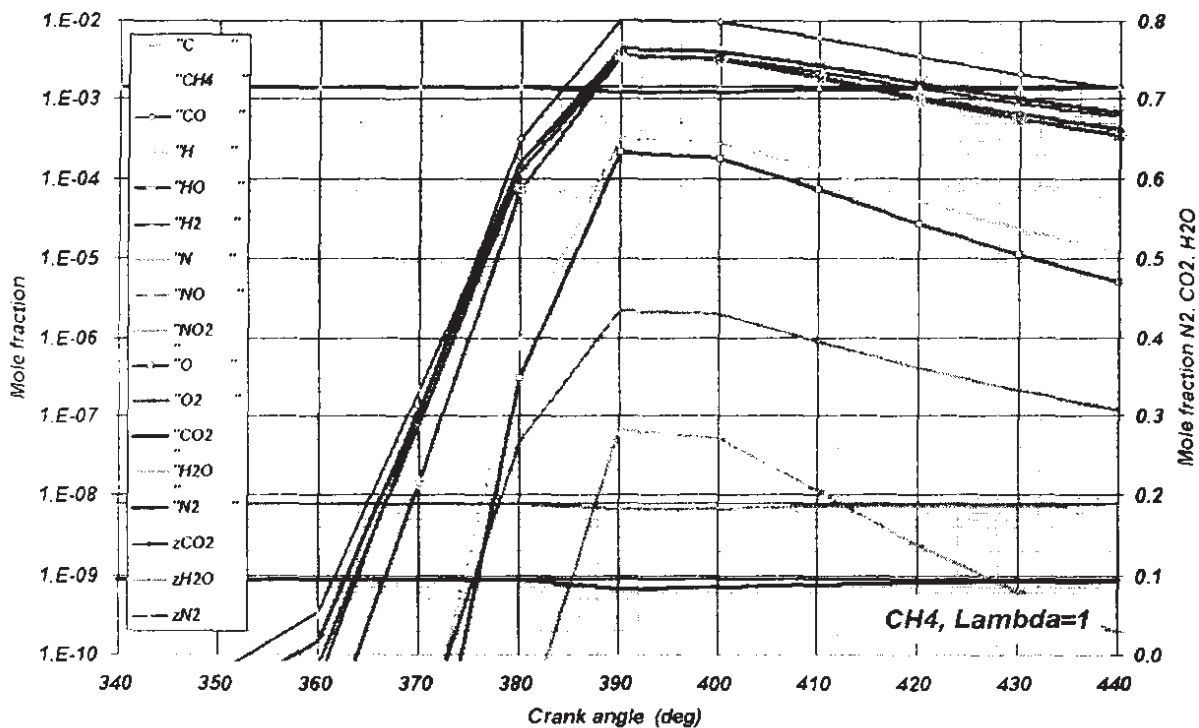
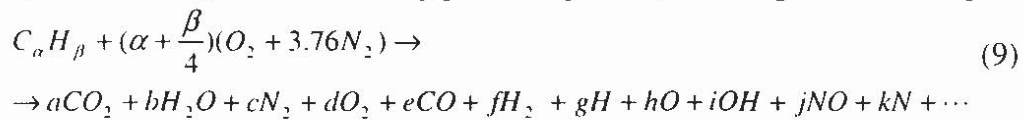


Fig. 4. Low temperature and Stanjan burnt gas compositions

For lean combustion we assume that there are no CO and H<sub>2</sub> in the product and for rich combustion we assume that there is no O<sub>2</sub> in the products. We assume also the equilibrium between the product species (water gas reaction  $CO_2+H_2=CO+H_2O$ ) with the equilibrium constant providing closing reaction [4,9].

In general, combustion process has many product species (including dissociation products):



The composition and hence the thermodynamic properties of the combustion reactants and products depend on thermodynamic state variables (p,T). After combustion the products of reaction are assumed to be in equilibrium. If temperature and pressure are given, the Gibbs free energy minimization is used. The Stanjan program [11] may be applied for that purpose. The results of the Stanjan calculations are shown in Fig.4 together with the results of Eq.8. It can be seen that the most significant differences between the compositions are observed in that range of crank angle in which temperature of working fluid is maximum.

#### 4. 1. Influence of product dissociation on C<sub>p</sub>/C<sub>v</sub> ratio

The influence of combustion products composition has been determined for both methane and iso-octane. Exhaust gas composition was calculated using Eq. 8 and Stanjan program (Fig.4). For these compositions the resultant specific heat ratios were calculated using equation:

$$\frac{1}{\kappa - 1} = \sum_{i=1}^k \frac{z_i}{\kappa_i - 1} \quad (z_i \text{ denotes the fraction of specie "i"}). \quad (10)$$

and the results presented in Fig. 5.

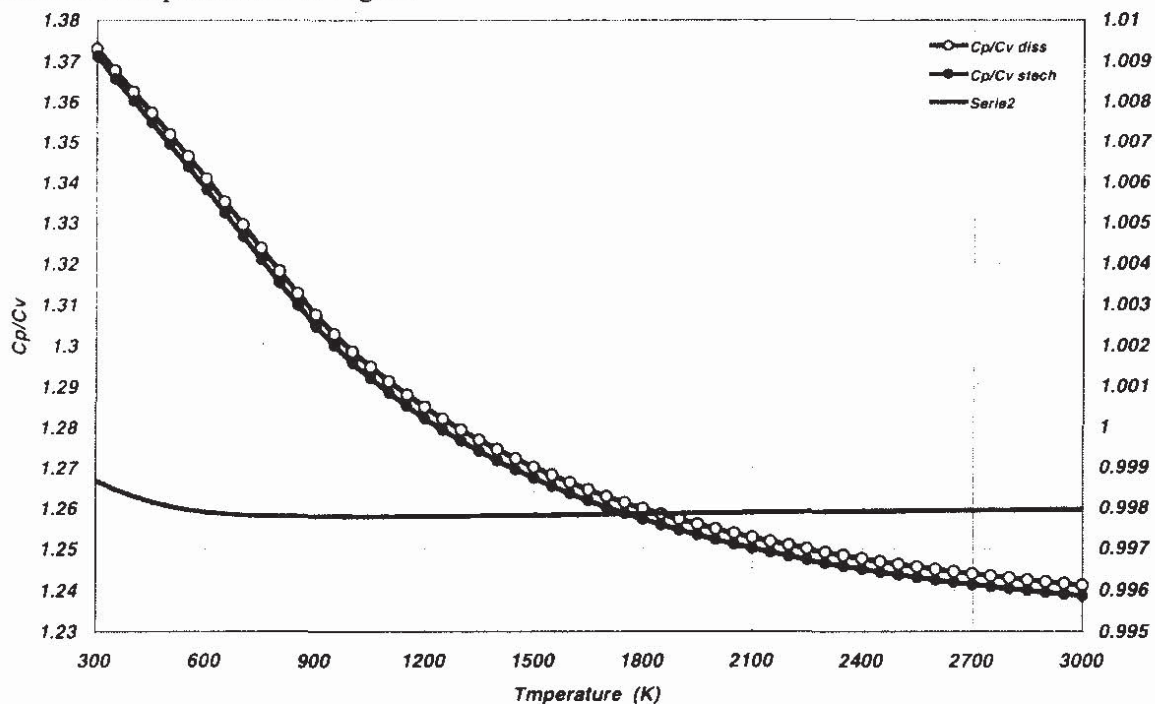


Fig. 5. Comparison of specific heat ratios calculated for stoichiometric low-temperature(Eq.8) and Stanjan burnt gas composition

From the figure we can see that there is no distinct difference between the C<sub>p</sub>/C<sub>v</sub> ratios for low temperature products and high-temperature dissociated ones.

## 4. 2. Influence of fuel properties

Specific heat ratios calculations were performed for stoichiometric ( $\lambda = 1$ ) mixtures of various engine fuels characterized by the H/C (hydrogen to carbon) ratios. The results (presented in Fig.6) indicate that the differences in  $C_p/C_v$  ratios are negligible.

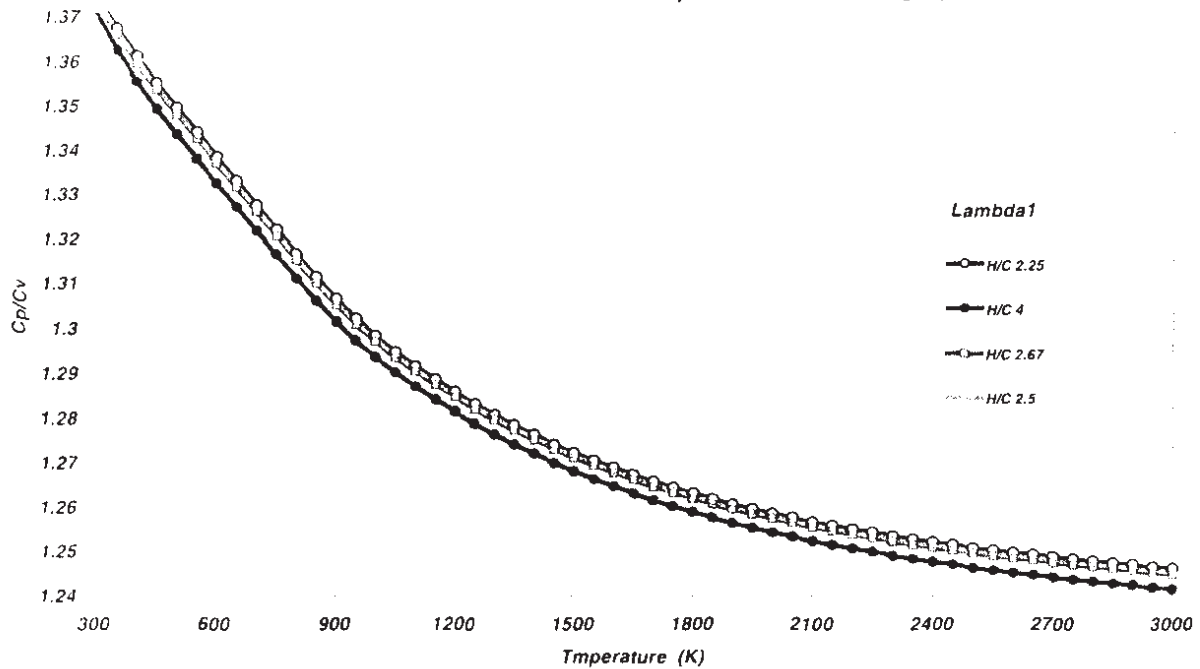


Fig. 6. Comparison of specific heat ratios calculated for different fuels (H/C=4 – methane, 2.87 – propane, 2.5 butane, 2.25 – isooctane)

## 4. 3. Influence of air excess

The influence of mixture strength was computed (for air-methane mixtures with air excess  $\lambda$  from 1 to 2) and illustrated in Fig. 7. Here we can observe that air excess changes can force larger effects: for maximum combustion temperature the differences in specific heat ratios of lean mixture can exceed 1 % (in relation to  $\lambda=1$ ).

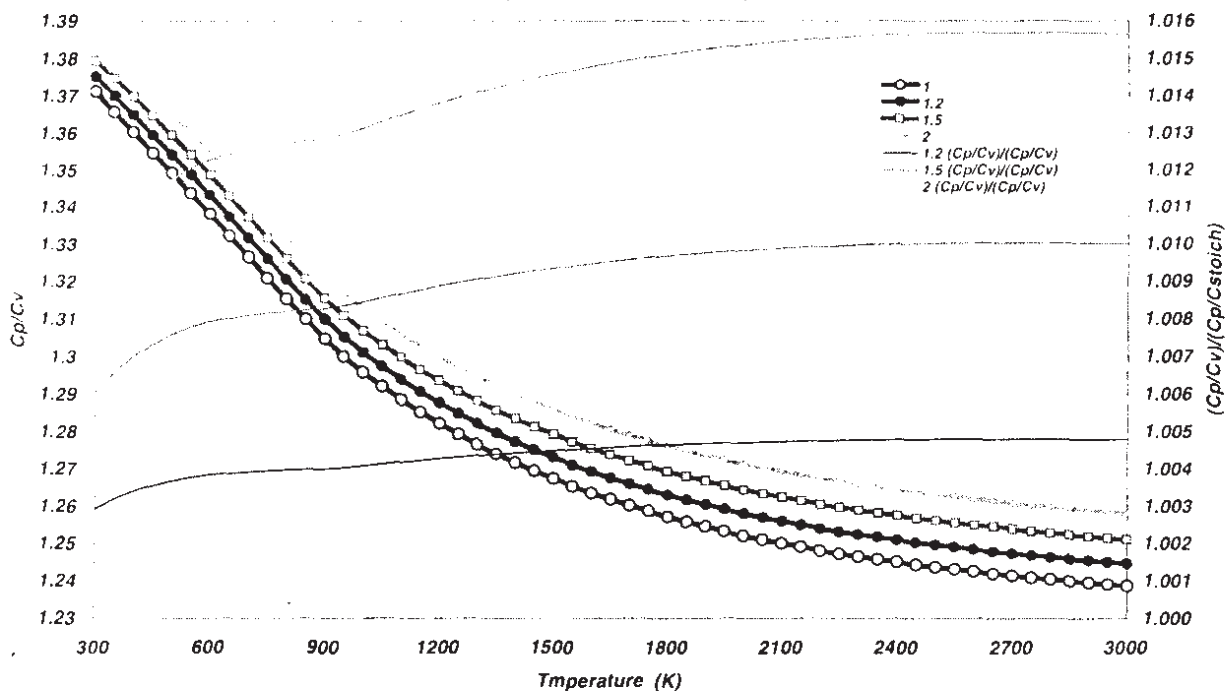


Fig. 7. Comparison of specific heat ratios calculated for different air excess ratios

## 5. Net heat release model

The traditional approach to the in-cylinder processes is based on the First Law of Thermodynamics and describes the heat release process according to the given cylinder pressure history. The thermodynamic model employed here follows that of Gatowski et al [3]. The content of the combustion chamber recognised as the control volume is regarded as a single working fluid and the combustion process is considered as an heat addition. Heat transfer through the cylinder boundaries and crevice flows are used to complete the energy balance.

The First Law of Thermodynamics applied to calculate the heat release rate (HRR) is as follows:

$$dQ_{ch} = dU_s + dW + dQ_{ht} + \sum h_{cv} dm_{cv} \quad (11)$$

Where:

$Q_{ch}$  -chemical energy of the fuel added to the working fluid during combustion;

$U_s$  -sensible internal energy;

$Q_{ht}$  -heat transferred from the working medium to the cylinder walls;

$h_{cv}$ ,  $m_{cv}$  -enthalpy and the mass flow to or from the crevices (or blow by).

When the chemical energy term  $dQ_{ch}$  is combined with heat transfer and crevice terms, we arrive at the final equation of net heat release rate:

$$\frac{dQ_{net}}{d\phi} = \frac{\kappa}{\kappa-1} p \frac{dV}{d\phi} + \frac{1}{\kappa-1} V \frac{dp}{d\phi} \quad (12)$$

This equation describes the incremental net HRR over a given crank angle interval during the period between IVC and EVO. The net heat release, performed on the measured in-cylinder pressure data, presents the heat effectively absorbed by working fluid.

For the analysis presented in this paper it was assumed that the calculations will be limited to two values of  $\kappa$ : "normal" one i.e. calculated according to the rules presented before and "speculative" one equal to 99% of the normal  $\kappa$ . The results of comparative calculations, shown in Fig.8, indicate that 1% difference in specific heat ratio can be the reason of 5% difference in net heat release rate.

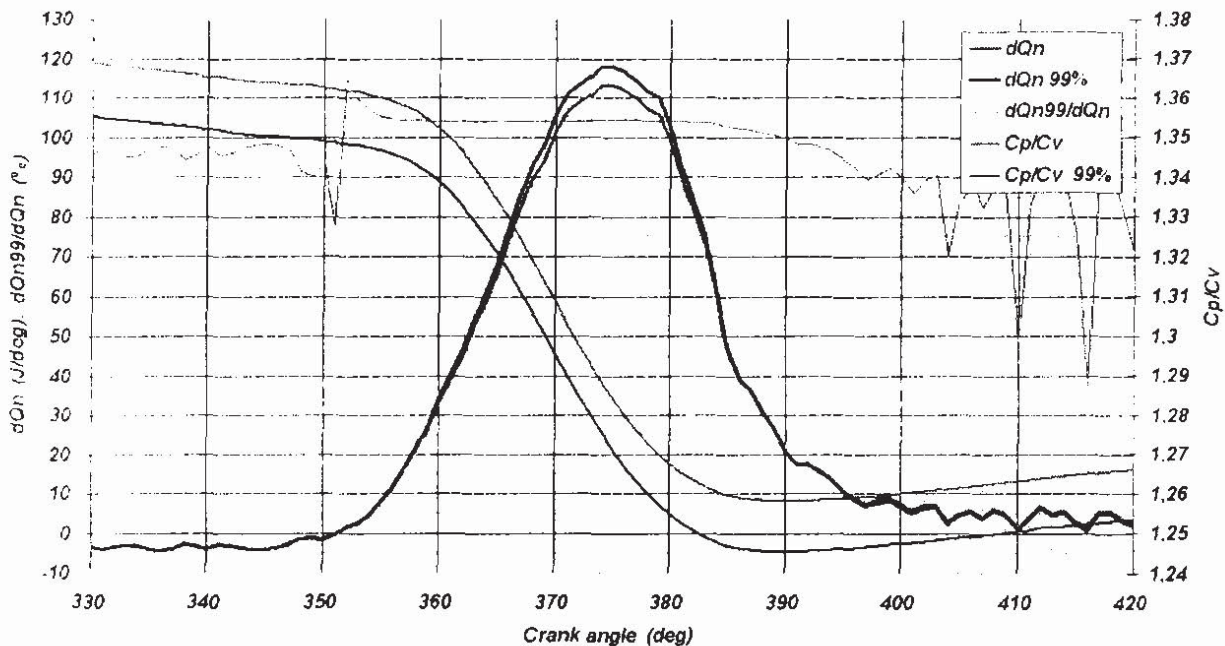


Fig. 8. Comparison of net heat release rates

## 6. Conclusions

Calculations of specific heat ratio for different kinds of engine working fluids has demonstrated that:

- effects of combustion products dissociation and fuel composition (H/C ratio) on  $C_p/C_v$  ratios are negligible;
- the changes of the proportions in fuel-air mixture have significant influence on  $C_p/C_v$  ratios and therefore should be taken into account when performing the heat release rate analysis.

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