AN ATTEMPT OF EXHAUST GASES COMPOSITION PREDICTION IN SI ENGINES POWERED BY PETROL AND GASEOUS FUELS

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Abstract

Optimization procedure of the si engines feeding systems requires the application of newer and more sophisticated tools, as an addition to well known but expensive experimental methods. Numerical methods can be considered nowadays as once playing the most important role in the combustion process analysis. Paper describes the application of the dual zone model, allowing the analysis of the combustion process in an SI engine with the possibility of estimating 10 different exhaust gases i.e.: CO_2, CO, H_2O, O_2, NO, N_2, H_2, H, O and OH. The research has been carried on a 1.6 litres four cylinder SI engine, fed with petrol and alternatively with LPG and CNG. In-cylinder pressure for the 4th cylinder of the tested engine has been acquired for several engine speeds. Registered in-cylinder pressure traces $p=p(\varphi)$, together with the volume variation $v_i=v_i(\varphi)$ in function of crank angle, were used in the combustion process simulating calculations. Obtained results made it possible to compare selected parameters describing the combustion process.

Obtained results do also prove recognized fact related to the higher temperature necessary to initiate gaseous fuel combustion.

Keywords: *CNG, LPG, exhaust gases, SI engine, combustion analysis*

1. Introduction

One of the most important topics of research in the Laboratory of Alternative Propulsion, part of the Department of Transport, is the use of alternative fuels in SI engines. Such fuels, e.g. natural gas, LPG and hydrogen, are attractive alternatives to the traditional fossil fuels like diesel and gasoline. Gaseous fuels are also less pollutant which related to conventional fuel featuring serious disadvantages concerning exhaust emissions: the noxious components such as nitrogen oxides (NOx), unburned hydrocarbons (UHC) and particulate matter pose a threat to human health and the environment.

Significant advantage of gaseous fuels is connected with lower then for conventional fuels CO_2 emission, extent responsible for the global warming of the planet. The major part of the research concerns hydrogen, the fuel that eliminates any harmful emissions (except NOx, which can be kept at very low levels), and of which there is an unlimited resource. This is an important advantage over fossil fuels, with their limited reserves. In recent years, several engines have been converted to operate on gaseous fuels. At the moment, the work has been focused on tree engines: a GM 1.6 liter L4 engine, GM 2.2 liter L4 and a one-cylinder research engine. The first and the second are intended to deliver knowledge concerning practical aspects that arise from preparing the engine for propulsion purposes. The third engine allows extensive research of the fundamental properties of the hydrogen combustion. All tests provided a lot of information on hydrogen propulsion, including economical aspects; an important disadvantage is the cost. At the moment, hydrogen is still expensive and thus, the tests have to be restricted in time. It is therefore very interesting to consider computer simulations which can be cost effective and give results in a considerably shorter time.

Spark ignition engine cycle simulation

The cycle of a four stroke SI engine consists of several parts: the intake of the fresh air-fuel mixture, the subsequent compression, ignition resulting in the combustion of the mixture, the expansion (power stroke) and finally the exhaust of the burned mixture.

The gasdynamic part, i.e. intake and exhaust, can be modeled with algorithms obtained from computational fluid dynamics (CFD). In the thermodynamic part, the simulation of the compression and expansion strokes are fairly straightforward following the laws of thermodynamics and some assumptions which accurately approximate the real processes. The most difficult part is the combustion simulation. The combustion process is a set of complicated events comprising turbulent flow and chemical reactions, of which a large part remains fairly unknown at this moment.

This uncertainty has led to a variety of simulation models. To simulate the combustion processes in a SI engine, one can follow different paths. The simplest option is a “zerodimensional” model, based on the first law of thermodynamics (conservation of energy). However, such a model requires several assumptions and can only give approximate results, due to its simplicity. On the other side of the spectrum of complexity, there are the multi-dimensional models. These consider the flow processes in the cylinder, the chemical kinetics and their interactions. The computation of these turbulent flows and their interaction with the combustion processes demand considerable computing power and CPU time, thus loosing some of the advantages of computer simulation. A compromise can be taken with a quasi-dimensional model. This is a model that takes some geometrical parameters into consideration and uses phenomenological models for the description of the turbulence and its interaction with the combustion process. Thus, a reasonable accuracy can be combined with fast computation. In order to model the physical and chemical processes that occur, it is necessary to distinguish the important events and parameters from the less important ones. This provides a deeper understanding of these processes.

Two-zone model

The quasi-dimensional model that has been chosen for the simulation of the combustion part in the thermodynamic cycle of a SI engine is a so-called “two-zone model”. This model is based on the model originally proposed by Wilk K. [13, 14], later adapted by numerous researchers as a better understanding of the occurring processes has been gained.

The simulation programme uses the model in the form developed by Tabaczynski et al. [5]. This model considers two zones in the combustion chamber: a zone with burned gases and a zone with the unburned mixture, divided by a spherical flame front. The combustion process is assumed to occur in two phases: first, unburned mixture is entrained into the flame front. In a second phase, this unburned mixture is burned. The combustion speed is calculated out of two differential equations. These take into consideration the characteristics of the turbulence in the combustion chamber and the laminar flame speed of the fuel (dependant of the pressure, temperature, amount of combustion air and residual gas). The combustion speed obtained with this model allows the evaluation of the equations determining the evolution of the pressure (assumed to be uniform throughout the cylinder) and the temperatures (uniform for each zone). These equations are derived from the first law of thermodynamics. A set of equations determines the composition of the cylinder gases by assuming chemical equilibrium at the given pressure and temperature.

Nowadays, mathematical models are often used to describe processes inside engine chamber. Mathematical models can be divided in two main groups according to heat release profile:

- individual model – heat release profile is based on indicated pressure,
- universal model – heat release profile is described by premised function (e.g. Wibe function).

Main advantage of universal model is the possibility of realizing combustion analyses, complete of all parameters. However, in this case it is necessary to premise the combustion angle start and combustion duration.

The proper way to a universal and reliable model is verification process of all functions which represent the combustion process and which have been acquired during tests on the engine bench. Verification methodology of the model which is has been presented in this paper is based on a balance of energy.

2. Measurement set-up

The original engine was Opel Astra naturally aspirated four cylinder petrol engine with displacement of 1.6 l with output of 55 kW at 5200 rpm and 128 Nm at 2600 rpm. This engine was modified for CNG fuelling without change in compression ratio. The engine was operated strictly stoichiometric and used one TW catalyst. Test procedure provided analysis at the idle and for selected higher RPM’s at the wide open throttle. Studies provided in-cylinder pressure registration in the crank angle domain for two different series. First series featured engine running on petrol, while the second one was registered for methane hydrogen mixtures operation. Experimental setup included pressure transducer type 6121, 2613B charge amplifier, crankshaft speed and position sensor DPA type by Kistler. Data were acquired through an eight channel NI board of the PCI-6143 type, driven by an application compiled in the LabView environment. Engine load variation was realized with the help of the BOSCH FLA 203 roller bench. Exhaust gases were registered by a fast response Pierburg HGA 400 5GR gas analyzer, while fuel consumption was measured respectively for petrol with the use of precise Pierburg PLU 401 device, while gaseous fuel consumption was registered by a tensometric balance. Experimental setup diagram has been presented on the Fig. 1.

Tab. 1. Main characteristics of the tested engine

Type	Four cylinder in-line
Displacement	1600 dm^3
Bore	79.0 mm
Stroke	81.5 mm
Compression ratio	9,6
Exhaust valve opening	41^o BTDC
Exhaust valve closing	11^o ATDC
Inlet valve opening	11^o BTDC
Inlet valve closing	41^o ATDC
EGR ratio	0 %

Registered for the tested engine in-cylinder pressure traces in the crank angle domain were the bases for further model calculations.

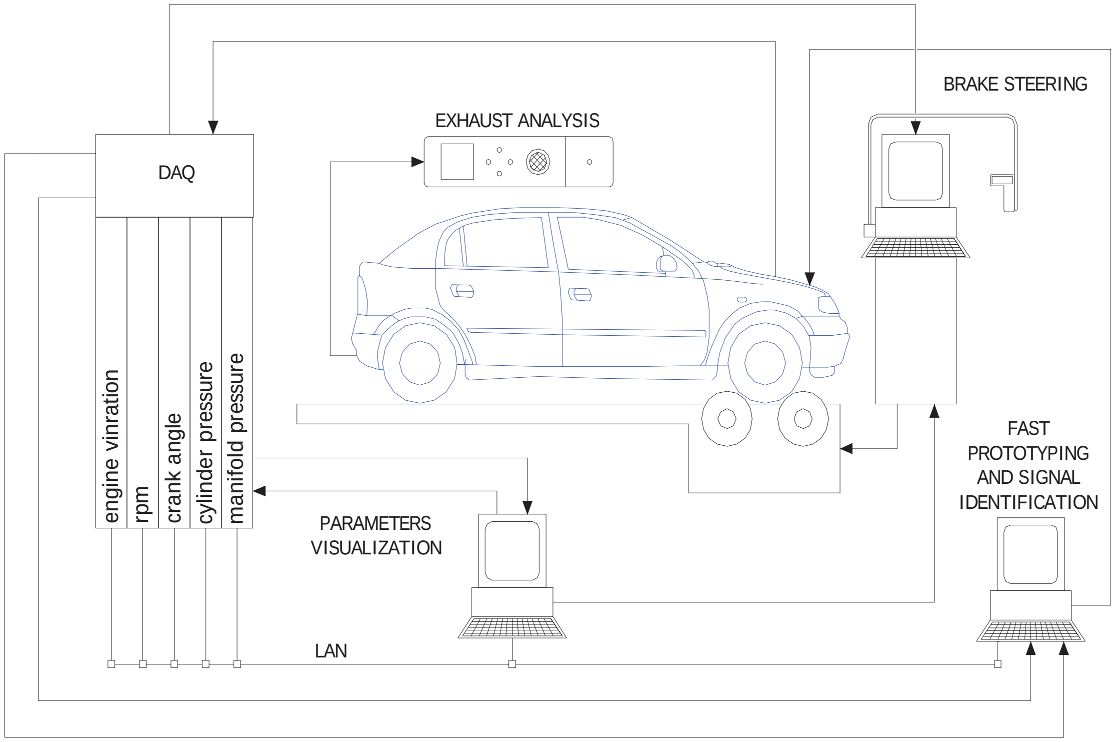

Fig. 1. Schematic diagram of experimental setup

Fig. 2. Engine comparment of tested vehicle

3. Dual zone model -description

Calculations carried on with the use of drawn up dual zone model, provided following assumptions:

- combustion chamber is being divided into two zones, separated by a infinitively thin flame front,
- temperature values in the zones are homogeneous,
- flame front temperature is equal to the exhaust gases temperature,
- air-fuel mixture and exhaust gases are qualified as semi ideal gases,
- chemical energy of air fuel mixture and exhaust gases (incompletely burned) is described by the calorific value.

Model has been described with the use of presented below equations, defined for elementary engine crank angle dφ:

- energy balance for the unburned mixture zone:

$$dQ = dU_u + dI_u + p * dV_u + dQ_{wu}\,, \tag{1}$$

- energy balance for the flame front:

$$dI_u = dI_b + dQ\,, \tag{2}$$

- energy balance for burned zone (exhaust gases):

$$dI_b = dU_b + p * dV_b + dQ_{wb}\,, \tag{3}$$

- thermal equation of the state of zones:

$$p * V_u = G_u * R_u * T_u\,, \tag{4}$$

$$p * V_b = G_b * R_b * T_b\,, \tag{5}$$

- equations of state for the substance quantity and volume:

$$G = G_u + G_b\,, \tag{6}$$

$$V_i = V_u + V_b\,, \tag{7}$$

- mass fraction burned:

$$x = \frac{G_b}{G}\,, \tag{8}$$

- fuel chemical energy release ratio:

$$y = x * \left(1 - \frac{W_{db}}{W_{du}}\right), \tag{9}$$

It has been also assumed, that exhaust gases as a product of the combustion process do constitute of an equilibrium solution consisting of ten components: CO_2, CO, H_2O, O_2, NO, N_2, H, O, OH, for the purposes of their mole fraction calculations the following were applied:

- Dalton's law

$$p_{i\,s} = (i) * p\,, \tag{10}$$

- equations of balances of elements of carbon C, hydrogen H, oxygen O and nitrogen N:

$$n_{C_f} = n_s^{''}\left[(CO_2) + (CO)\right], \tag{11}$$

$$\begin{aligned} &n_{H_f}^{'} + 2 * (H_2O)_a * \lambda * n_{a\,\min} = \\ &= n_s^{''}\left[2 * (H_2) + 2 * (H_2O) + (OH) + (H)\right], \end{aligned} \tag{12}$$

$$\begin{aligned} &n_{O_f}^{'} + \left[2 * (O_2)_a + (H_2O)_a\right] * \lambda * n_{a\,\min} = \\ &= n_s^{''}\left[(CO) + 2 * (CO_2) + 2 * (O_2) + (H_2O) + (O) + (NO)\right], \end{aligned} \tag{13}$$

$$n_{N_f}^{'} + 2 * (N_2)_a * \lambda * n_{a\,\min} = n_s^{''}\left[2 * (N_2) + (NO)\right], \tag{14}$$

- equation of the sum of fractions:

$$\begin{aligned} &(CO_2) + (CO) + (O_2) + (H_2) + (H_2O) + \\ &+ (OH) + (H) + (O) + (NO) + (N_2) = 1\,, \end{aligned} \tag{15}$$

- equations defining equilibrium constants K for the chosen reactions:

$$CO_2 \leftrightarrow CO + \tfrac{1}{2} O_2\,,\; K_1 = \frac{(CO) * (O_2)^{1/2}}{(CO_2)} * p^{1/2}\,, \tag{16}$$

$$H_2O \leftrightarrow H_2 + \tfrac{1}{2}O_2\,,\; K_2 = \frac{(H_2)*(O_2)^{1/2}}{(H_2O)} * p^{1/2}\,, \tag{17}$$

$$H_2O \leftrightarrow OH + \tfrac{1}{2}H_2\,,\; K_3 = \frac{(OH)*(H_2)^{1/2}}{(H_2O)} * p^{1/2}\,, \tag{18}$$

$$\tfrac{1}{2}H_2 \leftrightarrow H\,,\; K_4 = \frac{(H)}{(H_2)^{1/2}} * p^{1/2}\,, \tag{19}$$

$$\tfrac{1}{2}O \leftrightarrow O\,,\; K_5 = \frac{(O)}{(O_2)^{1/2}} * p^{1/2}\,, \tag{20}$$

$$\tfrac{1}{2}N_2 + \tfrac{1}{2}O_2 \leftrightarrow NO\,,\; K_6 = \frac{(NO)}{(N_2)^{1/2} * (O_2)^{1/2}}\,. \tag{21}$$

Equilibrium constants K, depending on the temperature were estimated according to the data listed in the [2]. Solving the equations, with the use of numerical method basing on the iteration for the selected variables range allowed the estimation of the temperatures both in the air-fuel mixture zone T_u, and in the exhaust gases zone T_b, as well as exhaust gases composition, all in the crank angle domain - φ.

Since equations defining energy balance for the burned and unburned mixture zones, and flame front are independent from dQ, there is no energy accumulation in the flame front, and equations can be transformed as follows:

$$0 = dU_u + dU_b + p * dV + dQ_w\,, \tag{22}$$

$$dI_b = dU_b + p * dV_b + dQ_{wb}\,. \tag{23}$$

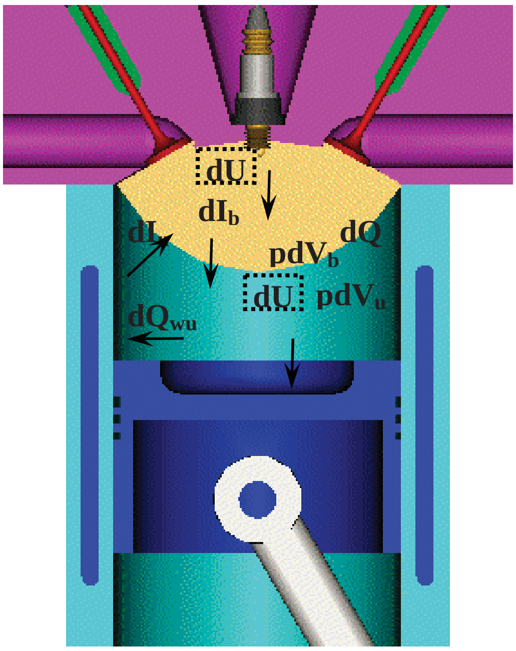

Fig. 3. Balance of energy for all zones

Entire enthalpy (physical and chemical) together with the charge and exhaust gases internal energy was taken into consideration, by adding to the calculations following equations:

$$u_u = W_{du} + \overline{c_{vu}} * \left(T_u - T_o\right) - R_u * T_o\,, \tag{24}$$

$$u_b = W_{db} + \overline{c_{vb}} * \left(T_b - T_o\right) - R_b * T_o\,, \tag{25}$$

$$i_u = W_{du} + \overline{c_{pu}} * \left(T_u - T_o\right), \tag{26}$$

$$i_b = W_{db} + \overline{c_{pb}} * \left(T_b - T_o\right). \tag{27}$$

Subsequent estimation of derivatives of charge internal energy, exhaust gases internal energy, charge enthalpy, exhaust gases enthalpy, heat transfer to the cylinder walls in the unburned zone, heat transfer to the cylinder walls in the exhaust gases zone, and mass fraction burned makes it possible to define equations allowing the calculation of:

- temperatures increments both in the unburned zone dT_u and in the exhaust gases zone dT_b,
- instantaneous temperatures T_u and T_b for every step of the calculation algorithm.

Working medium temperature mean value j was calculated with the use of the following equation:

$$T_{sr} = \frac{(1-x) * \overline{c_{vu}} * T_u + x * \overline{c_{vb}} * T_b}{(1-x) * \overline{c_{vu}} + x * \overline{c_{vb}}}. \tag{28}$$

For the calculation purposes an application named „EnComTwo" has been applied. Model verification has been done in the course of the research program connected with the combustion process analysis on the Perkins AD3.152G engine.

4. Model calculation results

Numerical calculations carried on the basis of a developed mathematical model made it possible to estimate and compare:

- mass fraction burned for engine running on petrol and alternatively on LPG and CNG, in the function of crank angle
- In-cylinder pressure and mass fraction burned increase for the engine running on petrol and gaseous fuels in the function of the crank angle,
- Maximum in-cylinder temperature, exhaust gases temperatures for the engine fed with petrol and gaseous fuel, in the function of engine crank angle
- Combustion process products both in the function of crank angle (in their formation process), as well as a summary value in the entire cycle.

Obtained results are presented in the Fig. 4 to 9.

Tab. 2 Results of calculation of temperature and parts of chosen exhaust product at the and of combustion

Fuel	Operating conditions			Combustion duration [dCA]	Temperature [K]			Emission			
									[%]		[ppm]
	Load	RPM	Ignition adv.		T_{bo}	T_{bmax}	T_{bs}	CO_2	CO	O_2	NO
Petrol	idle	800	10 dBTDC	87	2711	2711	1433	12.70	0.02	0.00	0.1
		4540	35 dBTDC	86	2314	3036	1501	12.63	0.09	0.04	52.8
	max	1520	30 dBTDC	86	2055	2543	1370	12.70	0.03	0.00	5.3
		2020	30 dBTDC	85	2069	2597	1333	12.70	0.03	0.00	2.4
		3000	35 dBTDC	87	2193	2945	1486	12.67	0.06	0.02	32.7
		4000	35 dBTDC	92	2182	2956	1446	12.67	0.05	0.01	29.4
LPG	idle	790	10 dBTDC	86	2723	2723	1591	11.17	0.06	0.64	332.1
		3940	35 dBTDC	101	2286	2739	1528	11.21	0.03	0.63	249.0
	max	1500	30 dBTDC	78	2186	2629	1501	11.22	0.01	0.62	217.6
		2000	30 dBTDC	78	2220	2862	1501	11.23	0.01	0.61	216.4
		3000	35 dBTDC	80	2023	2966	1906	11.11	0.02	0.56	526.3
		4000	35 dBTDC	80	1997	2932	1986	10.99	0.04	0.54	1188.0
CNG	idle	880	10 dBTDC	97	2654	2654	1777	9.10	0.02	0.38	516.9
		4270	35 dBTDC	82	2061	2626	1526	9.09	0.03	0.42	199.8
	max	1490	30 dBTDC	93	1936	2339	1525	9.10	0.02	0.43	200.5
		2010	30 dBTDC	82	1855	2346	1507	9.11	0.01	0.39	176.4
		2510	30 dBTDC	82	1849	2359	1518	9.11	0.01	0.39	185.7

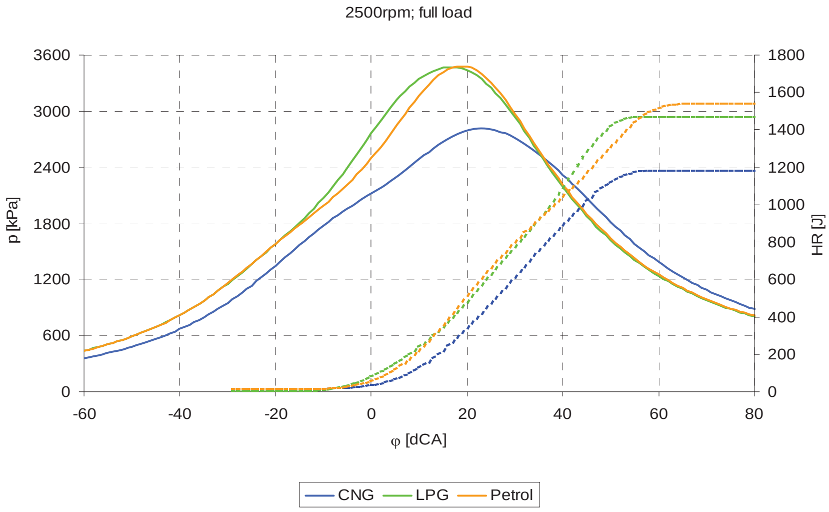

Fig. 4. In-cylinder pressure and heat released as a function of crank angle for tested engine (for rpm=2500 and full load)

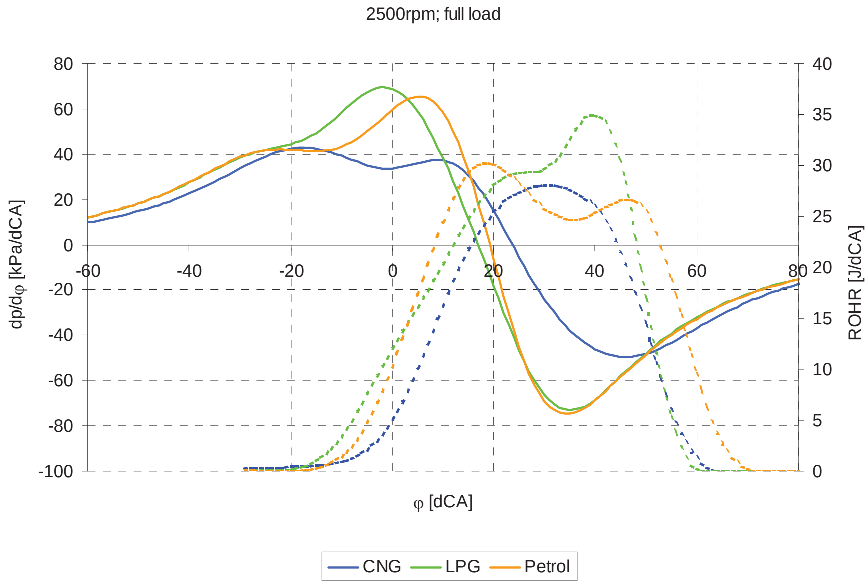

Fig. 5. Rates of pressure and heat released as a function of crank angle for rpm=2500 and full load

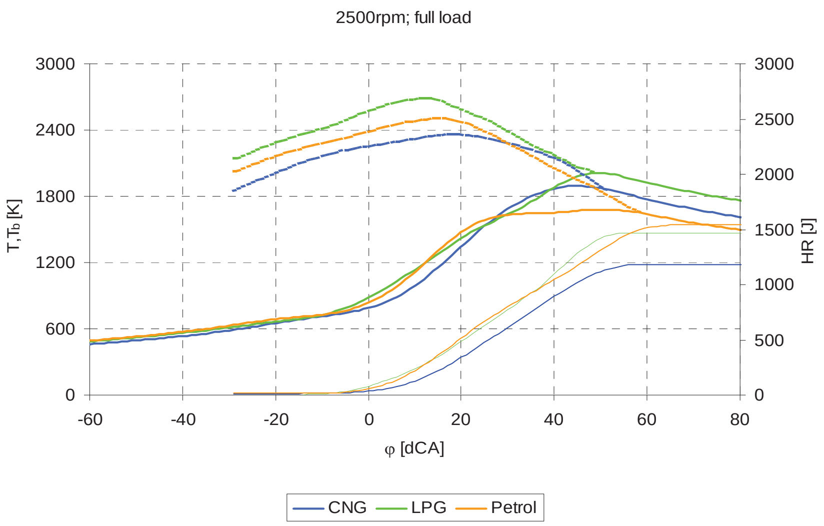

Fig. 6. In-cylinder temperatures and HR as a function of crank angle for rpm=2500 and full load

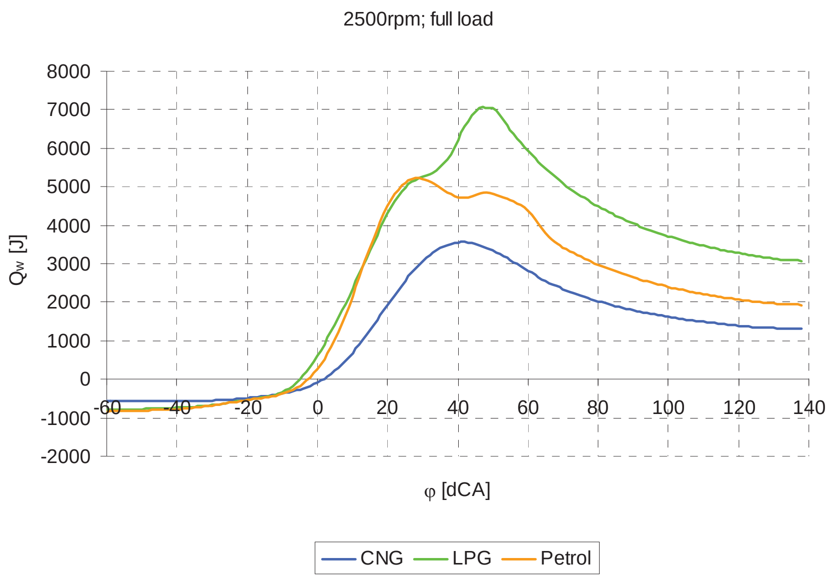

Fig. 7. Heat transferred between gases and chamber walls (rpm=2500, full load)

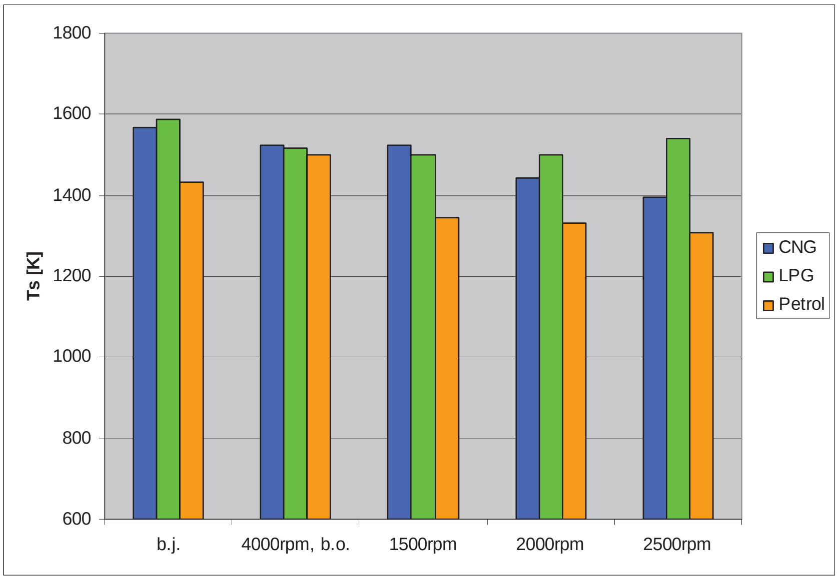

Fig. 8. An average gas temperatures in exhaust manifold (rpm=2500, full load)

4. Conclusion

Carried on simulations described in the paper, enabled the identification of differences between the combustion processes for gaseous fuels and petrol, which mainly relate to:

- different traces of the pressure and heat release in function of crank angle,
- different temperature traces registered for the charge combustion period,
- different charge combustion time,
- various mean temperatures levels for the combustion process and different quantities of the combustion process products.

Differences in the ROHR indicates, that the gaseous fuel combustion process develops longer, accelerating in its last phase. Petrol does combust with a constant speed.

The similar tendency can be observed for the temperature increase for the both of the tested fuels (Fig. 7 and 8). Gaseous fuels combustion phase lasts on average up to 20 degrees of the crank angle shorter.

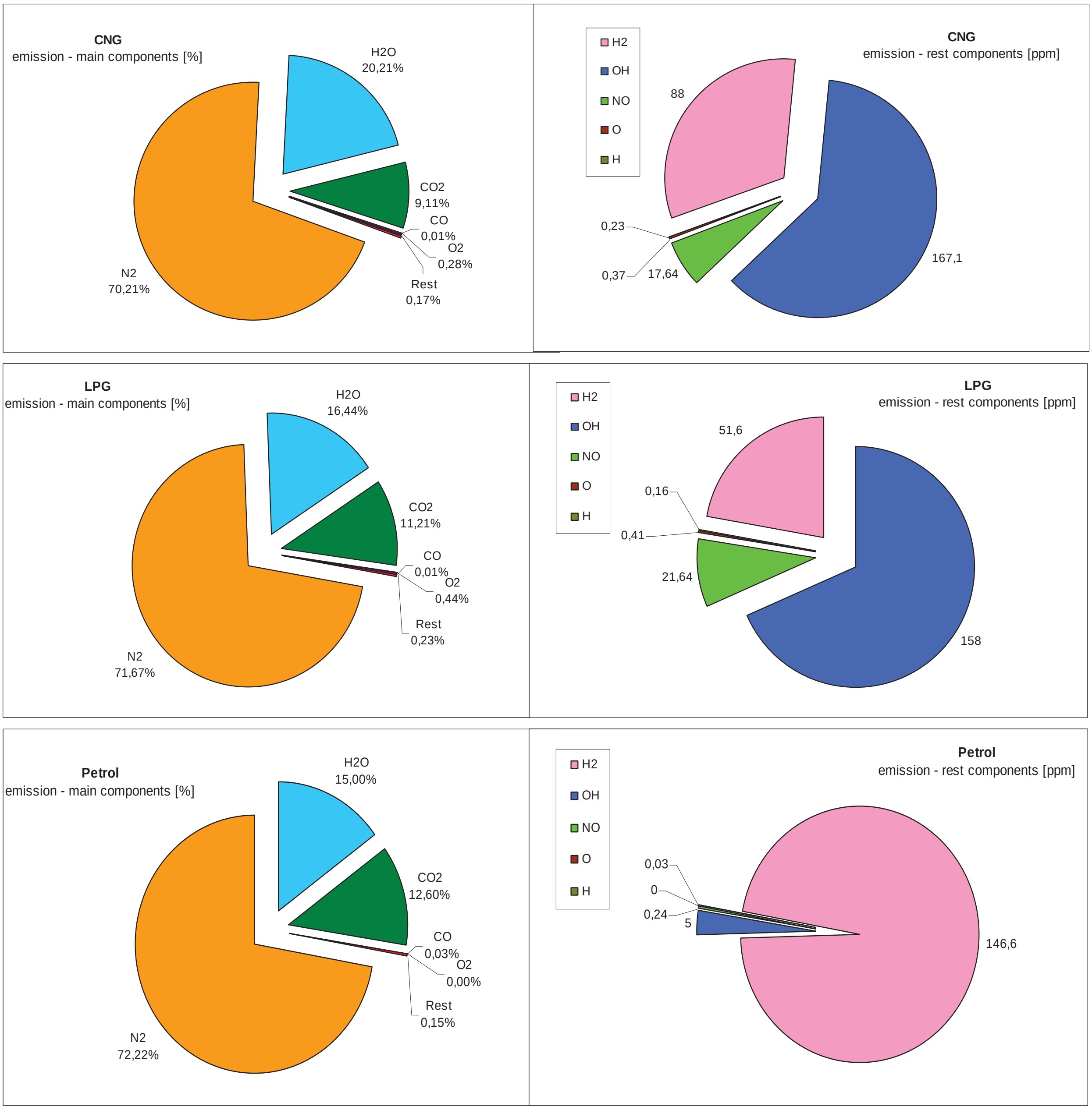

Fig. 9. Comparison of emitted gases composition

Registered temperatures values are higher in the case of gaseous fuel of about 400 K, what seriously influences the main exhaust gases levels in the combustion chamber.
Obtained results do also prove recognized fact related to the higher temperature necessary to initiate gaseous fuel combustion.

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Abbreviations

U_u, U_b	-	internal energy (chemical and physical) of the mixture and exhaust gases,
I_u, I_b	-	enthalpy (physical and chemical) of the mixture and exhaust gases,
T_u, T_b	-	temperature of the mixture and exhaust gases zone,
V_u, V_b	-	instantaneous volume of mixture and exhaust gases zone,
V_i	-	instantaneous volume of working area in the cylinder,
p	-	in-cylinder pressure,
Q	-	heat flowing to mixture zone from the flame front,
Q_{wu}, Q_{wb}	-	heat flowing to combustion chamber walls (engine head, piston, cylinder) from the mixture and exhaust gases zone,
G_u, G_b	-	weight if the mixture and exhaust gases per engine cycle,
G	-	charge weight per engine cycle,
X	-	mass fraction burned,
Y	-	fuel chemical energy release ratio,
W_{du}, W_{db}	-	mixture and exhast gases calorific value,
$n_{C_f}, n_{H_f}, n_{O_f}, n_{N_f}$	-	number of kilomoles of C, H, O i N in the fuel related to the fuel unit,
$n_s^{"}$	-	number of kilomoles of humid exhaust gases related to a fuel unit,
$n_{a\,\min}$	-	theoretical air kilomoles demand for the fuel unit combustion,
λ	-	air excess ratio,
P_{is}	-	partial pressure of a i component of the exhaust gases.