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Computer simulation of SI engine fuelled with different fuels

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In order to evaluate the influence of the kind of fuel on combustion parameters and engine overall efficiency, simple simulation model of combustion in SI engine has been developed. Computations performed for gasoline, methanol and ethanol revealed that for methanol application, engine overall efficiency is the highest, as well as pressure, temperature in the cylinder and the rate of burning of the charge.

1. Introduction

Modelling of combustion processes in IC engine has become a useful tool that permits predicting of engine behaviour in a wide range of its operating parameters and design variables. There are many models, more or less complicated, that can be used for computation of combustion parameters and emission of IC engine, as, for instance, these, which constitute the base for KIVA programme and others [1].

However, the models of high generality levels are too complicated for solving not so much refined phenomena, for which simple models not demanding big and expensive computers may be used.

The objective of this paper is to evaluate the kind of fuel on engine combustion and on its operating parameters, especially thermal efficiency.

A simple simulation model of combustion in SI engine has been developed, which enables valuation of the influence of different kinds of fuels on the pressure and the temperature time history in engine cylinder during combustion, engine overall efficiency and brake torque. It also enables to estimate the influence of the main engine regulating parameters – ignition advance, mixture strength etc. – on above mentioned phenomena.

The model is zero-dimensional, heat release is assumed to be described by Viebe-function. This model has been assumed, because it is very simple zero-dimensional and general (i.e. not related to any combustion system) and – due to that – may be used for engine being designed at the moment. In the model and thermodynamic gas properties are functions of temperature and gas composition. Computational programme has been developed and computations have been performed.

Analysis of the influence of three fuels: gasoline, methanol and ethanol and engine operating and regulating parameters on combustion parameters has been performed.

2. Description of the model

2.1. Main assumptions

Main assumptions of the physical model of combustion processes in the engine cylinder are as follows.

- The model is zero-dimensional, it means that throughout of the gases the pressure and temperature are uniform.
- Gases in the cylinder are always in thermodynamic equilibrium.
- As we are interested in the processes of combustion, the mass of gases in the cylinder can be assumed to be constant, i.e. the valves are closed and there is no leakage to the crank-case.
- The gases fulfil the Clapeyron's equation (of the state).
- The fraction of burnt fuels is described by Viebe-functions [2].
- The calorific parameters of gases, i.e. specific heats and enthalpies, are described by McBride's relation.
- The heat of combustion is equal to the change of internal energy of the gas.
- For determinations of heat transfer to the walls, Hohenberg's relation is used.
- Friction losses are determined by Thiele expression.
- Work of charge exchange is determined with the use of assumed difference of the pressure at the end of expansion and suction pressure.

2.2. Governing equation

The equation of the first low of thermodynamics for closed system (constant mass, m) and uniform pressure and temperature throughout the gas being in thermodynamic equilibrium:

$$\frac{d(m\cdot u)}{d\varphi}=\frac{dQ}{d\varphi}-p\frac{dV}{d\varphi}-\frac{dQ_w}{d\varphi} \tag{1}$$

Number of moles of the gas, i.e. air and fuel vapour in the cylinder:

$$n=\eta_V\cdot\frac{p_o\cdot V_s}{B\cdot T} \tag{2}$$

Number of moles of the air in the cylinder:

$$n_{\text{air}}=\eta_V\cdot\frac{p_o\cdot V_s}{B\cdot T\cdot\left(1+\dfrac{\mu_{\text{air}}\cdot f_V}{\lambda\cdot\sum\limits_{(i)} f_i\cdot L_{oi}}\cdot\sum\limits_{(i)}\dfrac{f_i}{\mu_i}\right)} \tag{3}$$

where:

f_i – mass fraction of each fuel i in the fuel mixture,

μ_i – molecular weight of each i in the fuel mixture,

f_v – mass fraction of the evaporated (entire fuel mixture),
L_{oi} – stoichiometric air/fuel ratio, kg air/kg fuel, for each fuel i.

Clapeyron's equation of the gas:

$$pV = nBT \tag{4}$$

Universal gas constant and polytropic exponent:

$$k = \frac{c_p}{c_v} \tag{5a}$$

$$B = c_p - c_v \tag{5b}$$

Internal energy and enthalpy fulfil the equation:

$$u(T) = h(T) - BT \tag{6}$$

Fraction of the burnt gas:

$$x = 1 - \exp\left[C\left(\frac{\varphi - \varphi_{bc}}{\varphi_{ec} - \varphi_{bc}}\right)^{m+1}\right] \tag{7}$$

where:
m – exponent
C – constant,

$$C = \ln(1 - x_C), \quad x_C = 0.99 \tag{8}$$

φ – actual crank angle,
φ_{bc} – crank angle for beginning of combustion,
φ_{ec} – crank angle for the end of combustion.

Molar specific heat by $P = \text{const}$ for each species i [3]:

$$c_{pi} = B \cdot (a_{i1} + a_{i2}T + a_{i3}T^2 + a_{i4}T^3 + a_{i5}T^4) \tag{9}$$

Molar specific enthalpy for each species i [3]:

$$h_i = BT\left(a_{i1} + \frac{1}{2}a_{i2}T + \frac{1}{3}a_{i3}T^2 + \frac{1}{4}a_{i4}T^3 + \frac{1}{5}a_{i5}T^4 - \frac{a_{i6}}{T}\right) \tag{10}$$

Vapours of the fuels:

$$c_{pf} = (A_{f1} + A_{f2}t + A_{f3}t^2 + A_{f4}t^3 + A_{f5}t^{-2}) \tag{11}$$

$$h_f = t\left(A_{f1} + \frac{1}{2}A_{f2}t + \frac{1}{3}A_{f3}t^2 + \frac{1}{4}A_{f4}t^3 - \frac{A_{f5}}{t}\right) + A_{f6} + A_{f8} \tag{12}$$

where:

$$t = \frac{T}{1000}$$

Constant values in Eq. (9)−(12) can be taken from literature, e.g. [3]. Other than c_p and h thermodynamic gas and fuel vapour properties can be computed by the use of above equations. Heat released during combustion (calorific value of the mixture) is defined as a difference of absolute internal energy [3]:

$$W(T) = -\Delta u(T) = u_b(T) - u_e(T) \tag{13}$$

where:

$u_b(T)$ — internal energy at the beginning of combustion,
$u_e(T)$ — internal energy at the end of combustion.

Internal energy u is the function of temperature and gas composition. In Eq. (13) the amount of energy released depends on the conditions at which energy is released, i.e. instantaneous temperature level and gas composition; in normal conditions it is defined as fuel calorific value, c_v.

Coefficient of heat transfer from gases to walls is expressed by Hohenberg's relation [4]:

$$\alpha = 130\, V^{-0.06} p^{0.8}\, T^{-0.4} (c_m + 1.4)^{0.8} \quad \left[\frac{\mathrm{W}}{\mathrm{m^2K}}\right] \tag{14}$$

where:

c_m — mean piston speed, m/s, defined as follows

$$c_m = \frac{s \cdot n}{30} \tag{15}$$

V, p, T — are instantaneous volume of the cylinder above piston in m^3, pressure in bars and temperature in kelvins, respectively.

Coefficient of thermal conductivity through the wall is defined by well known equation:

$$k = \frac{1}{\dfrac{1}{\alpha_w} + \dfrac{\delta}{\lambda_s}} \tag{16}$$

where:

δ — wall thickness,
λ — thermal conductivity of the material of cylinder wall,
α_w — coefficient of heat transfer from the walls to cooling water.

Cefficient of heat transfer from the walls to cooling water is expressed by equation given by Wanscheidt [5].

$$\alpha_w = 35 + 2100\sqrt{w}, \quad \left[\frac{\mathrm{W}}{\mathrm{m^2K}}\right] \tag{17}$$

where:

w — is velocity of cooling water, m/s.

Heat transferred to the walls is described by the following expression:

$$\frac{dQ_w}{d\varphi}=\frac{\sum_i A_i(T-T_{mi})\alpha}{6\cdot n\cdot dt} \tag{18}$$

where:

T – instantaneous temperature of the gas in the cylinder,
A_i – area of heat transfer,
T_{mi} – mean temperature of the i wall surface expressed by relation

$$T_m=\frac{\alpha T+kT_l}{\alpha+k} \tag{19}$$

where:

T_l – temperature of the cooling liquid,
α – heat transfer coefficient,
k – thermal conductivity through the wall, Eq. (16),
T, α – as in Eq. (18).

2.3. Further evaluation of basic equations and computational procedure

Temperature can be determined from Eq. (1), under the assumption, that the gas in the cylinder is ideal, $u=u(T)$ and

$$du=c_v dT \tag{20}$$

Eq. (1) may be expressed in the form:

$$\frac{dT}{d\varphi}=\frac{1}{c_v m}\left(\frac{dQ_B}{d\varphi}-\frac{dQ_W}{d\varphi}-p\frac{dV}{d\varphi}\right) \tag{21}$$

Heat released during combustion is:

$$\frac{dQ_B}{d\varphi}=m\frac{dx}{d\varphi}W(T) \tag{22}$$

where:

$W(T)$ – is defined by Eq. (13).

Pressure and temperature always fulfil equation of state, Eq. (4). So taking into account Eq. (4), Eq. (21) and Eq. (22) may be combined together and written in the form:

$$\frac{dT}{d\varphi}=\frac{1}{c_v m}\left(m\frac{dx}{d\varphi}W(T)-\frac{dQ_W}{d\varphi}-\frac{nBT}{V_s}\frac{dV}{d\varphi}\right) \tag{23}$$

All terms in this equation, as well a $\frac{dV}{d\varphi}$ can be computed in each computational step.

Eq. (1) enables computation of temperature vs. φ. Pressure time history in the cylinder can be then obtained from Eq. (4). The computational programme has been worked out. The computational procedure is described in Appendix 1.

Friction losses can be the use of friction pressure, expressed by Thiele equation, valid for $p_{fr} \leqslant 4$ bars:

$$p_{fr} = 6.7 \times D^{-0.329} - 89 \times D^{-0.943} \times \left(1 - \frac{n}{n_N}\right) \tag{24}$$

where:

D – cylinder diameter, mm,
n – engine speed, rpm,
n_N – engine speed at maximum power, rpm.

The above mentioned equation takes into account flor losses and the power of peripheral equipment.

The charge exchange work per cycle is expressed by the equation:

$$L_{ch.exch.} = (p_4 - p_1) \cdot V_s = \Delta P \cdot V_s \tag{25}$$

where:

p_4, p_1 – cylinder pressure at the end of expansion stroke and the begining of filling stroke.

Equation (23) doesn't take into account dynamic flow losses. In order to obtain effective engine performances, e.g. mean effective pressure, p_e and effective engine efficiency, friction losses and charge exchange losses should be taken into account.

The computational procedure is supplied with algorithm correcting parameters of Wibe function proposed by Szczęsny [6].

Computations were performed for two kinds of gasoline and two alcohols: methanol and ethanol.

3. Results of computations

3.1. Influence of kind of fuel

The influence of the kind of fuel on pressure, temperature and fraction of burnt fuel vs. actual cylinder volume and crank angle, respectively are shown in Fig. 1 to Fig. 3. From these figures it may be deduced that fuelling with methanol gives reasonable pressure, the highest maximum temperature and the biggest work (Fig. 1). These lead to maximum engine overall efficiency, which is shown vs. ignition advance in Fig. 4 and vs. air excess coefficient, Fig. 5.

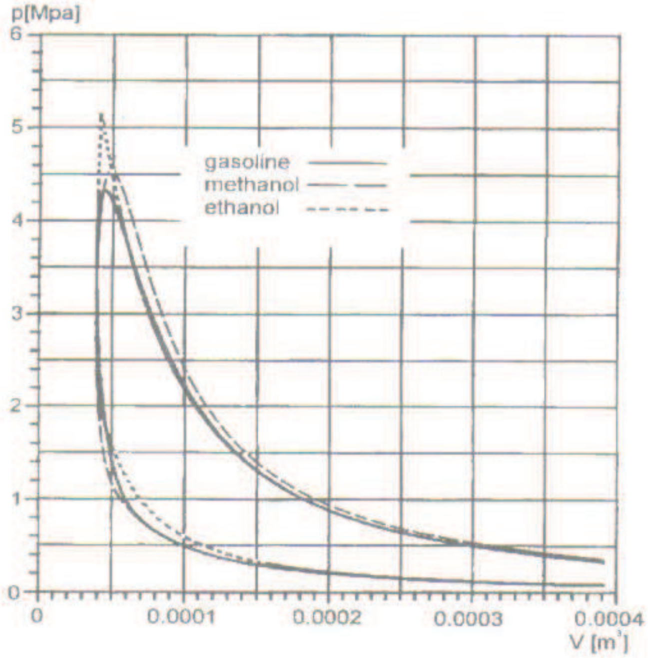

Fig. 1. Indicator diagram for engine fuelled with gasoline, ethanol and methanol. Ignition advance optimized for max. efficiency. $\eta_v = 0.8$, $\lambda = 1.0$, $n = 2500$ rpm

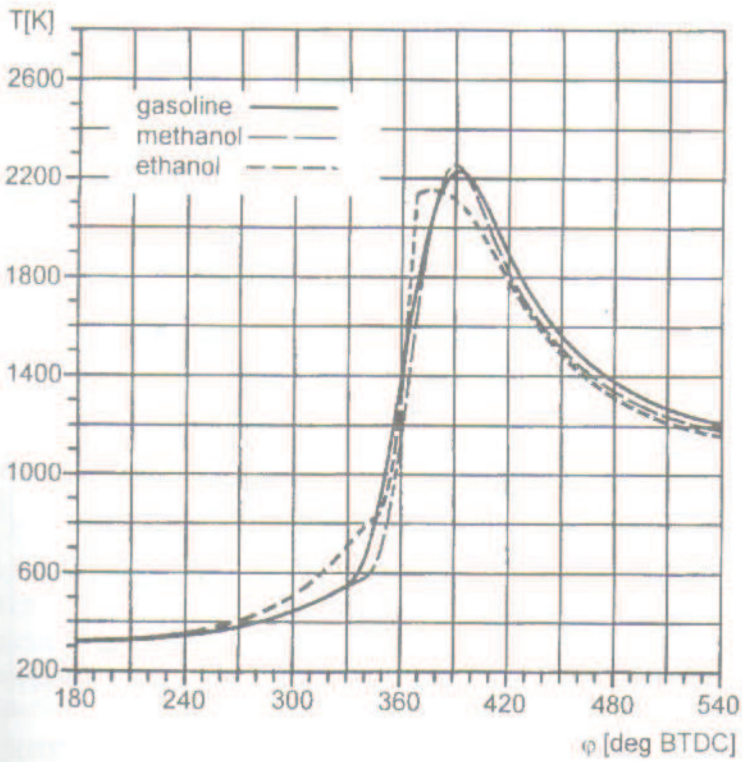

Fig. 2. Temperature of the gas in the cylinder vs. crank angle. Conditions as in Fig. 1

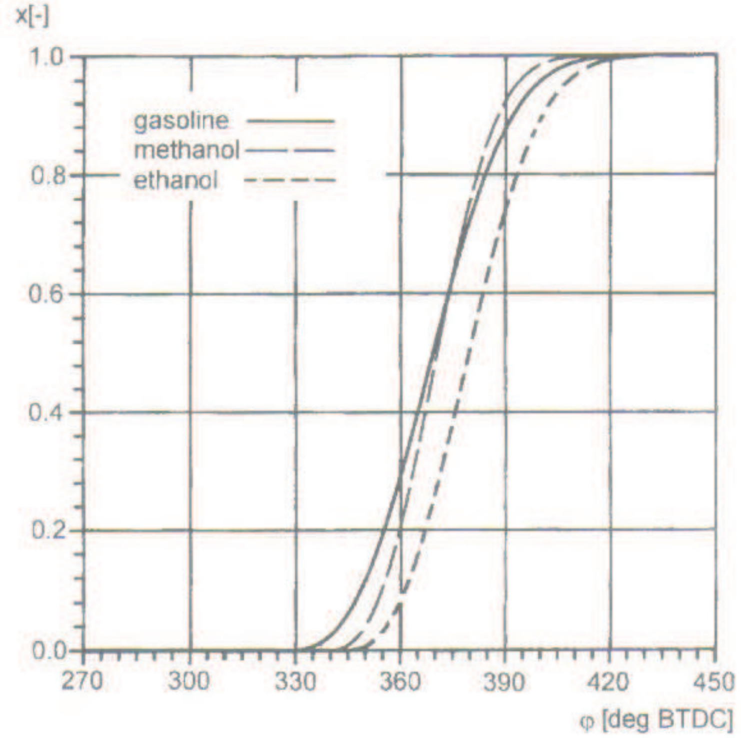

Fig. 3. Fraction of burnt fuel vs. crank angle. Conditions as in Fig. 1

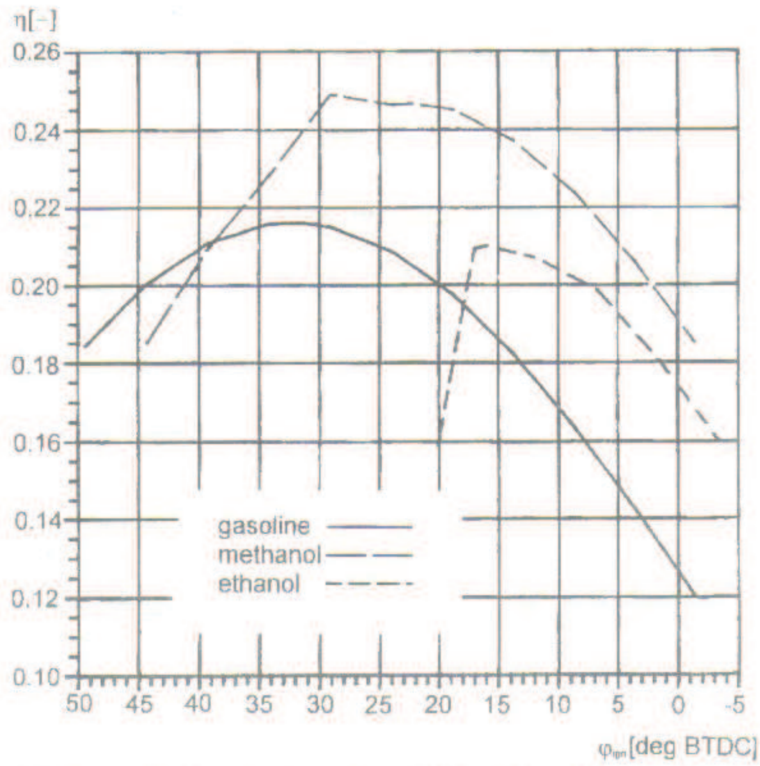

Fig. 4. Engine efficiency vs. ignition advance angle. $\eta_v = 0.8$, $\lambda = 1.0$, $n = 2500$ rpm, 20% of fuel evaporated

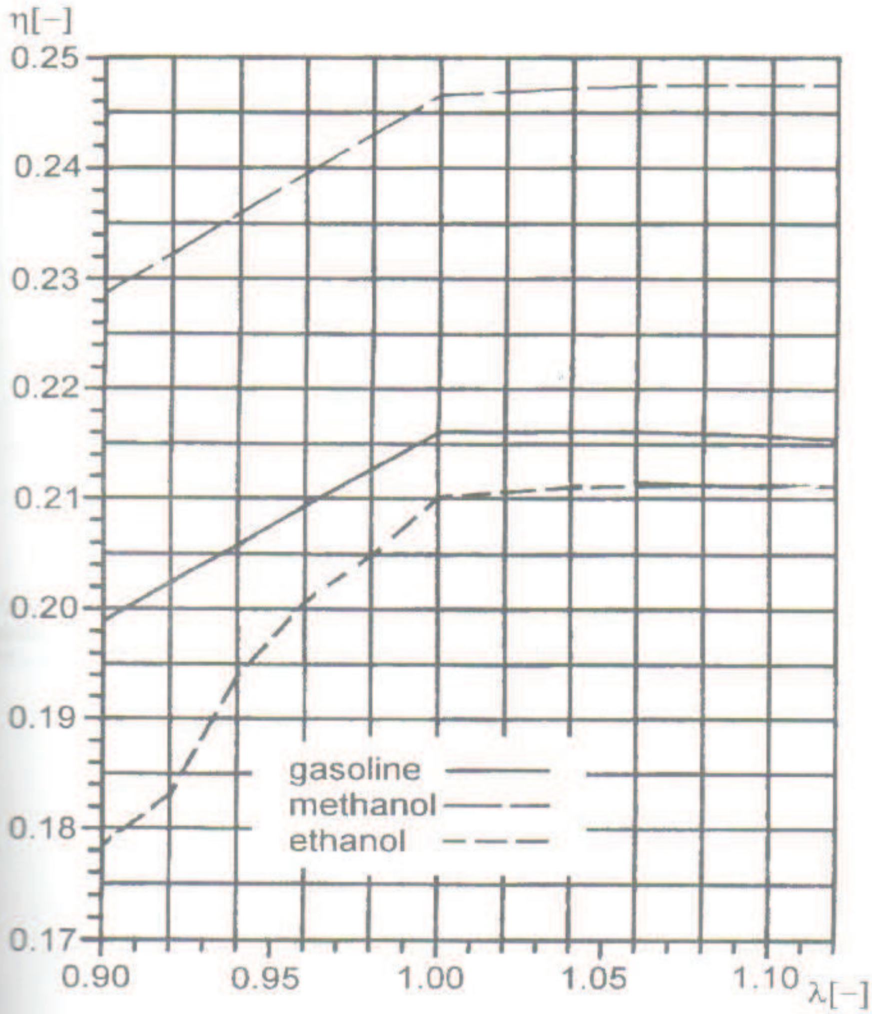

Fig. 5. Engine efficiency vs. coefficient of air excess. Conditions as in Fig. 4

3.2. Influence of ignition advance

The influence of the ignition advance on pressure and temperature vs. crank angle are shown in Fig. 6 and Fig. 7 for gasoline and in Fig. 8 and Fig. 9 for methanol, respectively. From these figures it may be seen that:

- optimal ignition advance on account on engine efficiency for gasoline ($\varphi_z \approx 33$ deg BTDC) is greater that for methanol ($\varphi_z \approx 22$ deg BTDC),
- maximum pressure and maximum temperature for both fuels is almost the same,
- methanol is much more sensitive for ignition advance than gasoline,
- late ignition for methanol results in break-down of pressure behind TDC (Fig. 8),

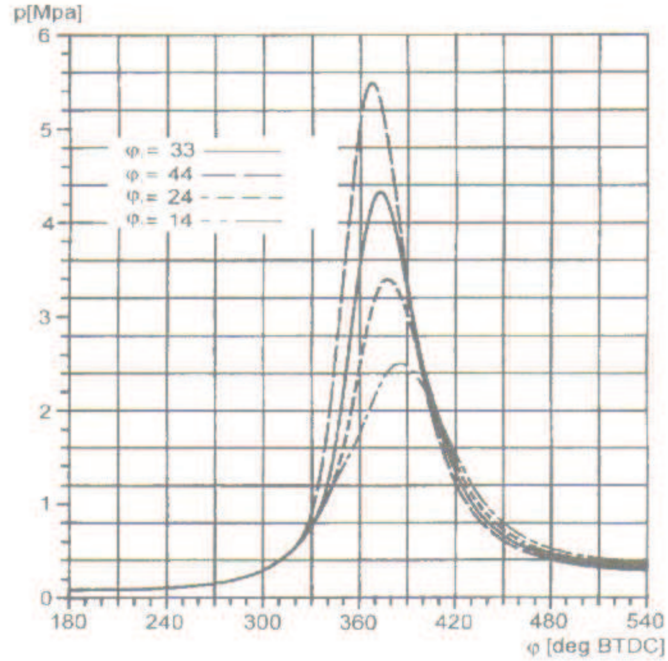

Fig. 6. Pressure in the cylinder vs. crank angle for different spark timings for engine fuelled with gasoline. Ignition advance optimized on account on engine efficiency 33 deg BTDC. $\eta_v = 0.8$, $\lambda = 1.0$, $n = 2500$ rpm

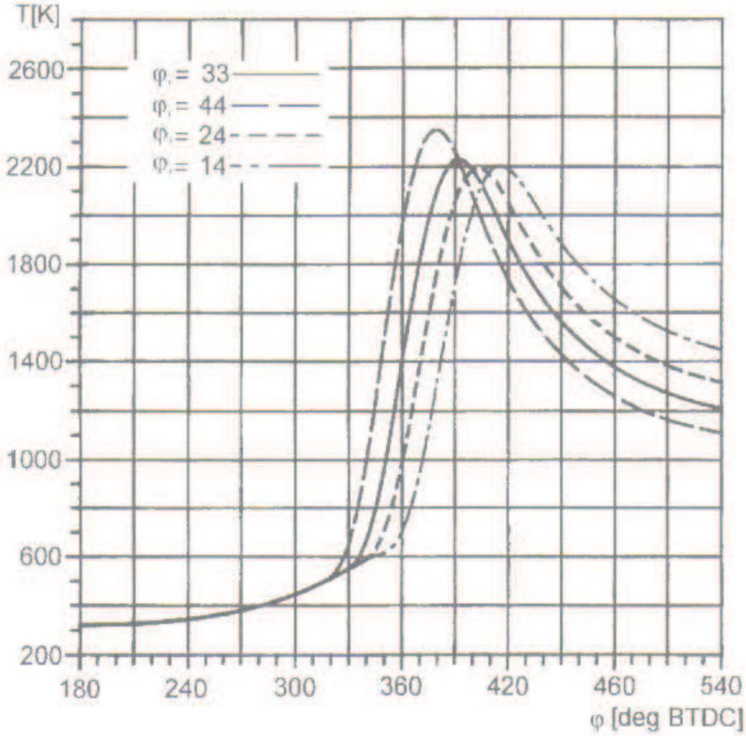

Fig. 7. Temperature of gases in the cylinder vs. crank angle for different spark timings. Conditions as in Fig. 6

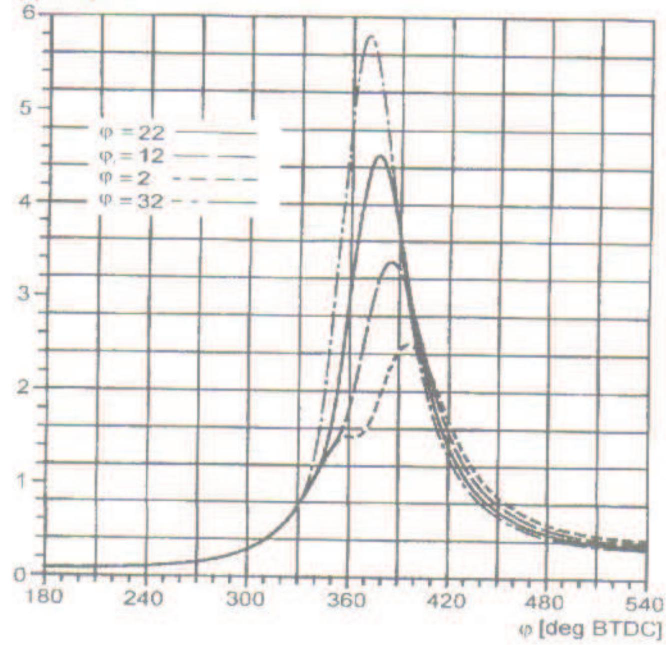

Fig. 8. Pressure in the cylinder vs. crank angle for different spark timings for engine fuelled with methanol. Ignition advance optimized on account on engine efficiency 22 deg BTDC. $\eta_v = 0.8$, $\lambda = 1.0$, $n = 2500$ rpm

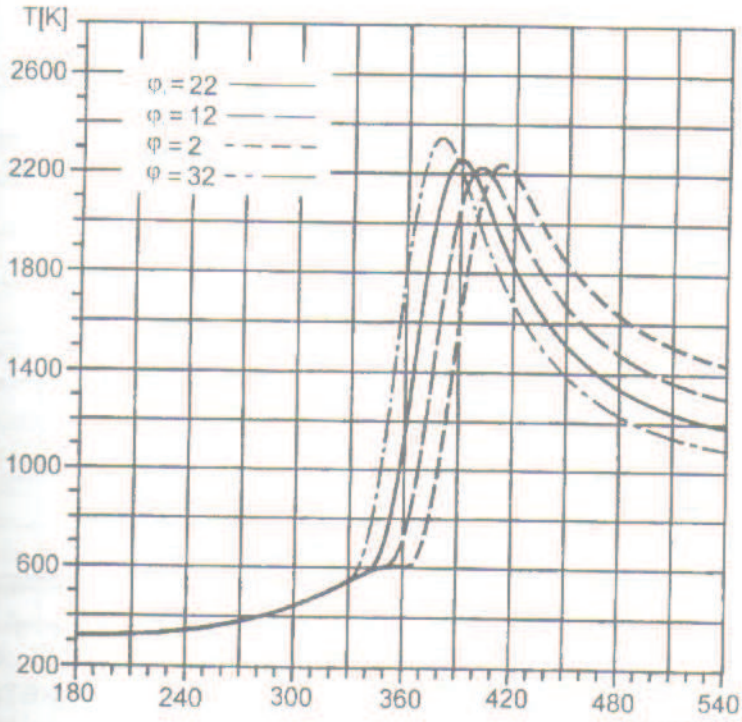

Fig. 9. Temperature of gases in the cylinder vs. crank angle for different spark timings. Conditions as in Fig. 8

– for approximately the same ignition advance, maximum pressure is higher for methanol than for gasoline (Fig. 6 and Fig. 8) while maximum temperature is almost at the same level (Fig. 7 and Fig. 9).

The influence of ignition advance on efficiency is shown in Fig. 4. From this figure it may be concluded that alcohols are more sensitive for ignition advance than gasoline, especially ethanol, which is more sensitive than methanol.

3.3. Influence of air-fuel ratio

The influence of the mixture air-fuel ratio on pressure and temperature of gases in the cylinder are shown in Fig. 10 and Fig. 11 for engine fuelled with gasoline. As may be seen, temperature gest its maximum for $\lambda=0.8$, i.e. for reach mixture, while pressure – for stoichiometric one. From Fig. 5 it may be seen, that maximum engine efficiency has been reached for $\lambda=1.1$ for methanol fuelling, while for gasoline – for $\lambda\approx1.05$.

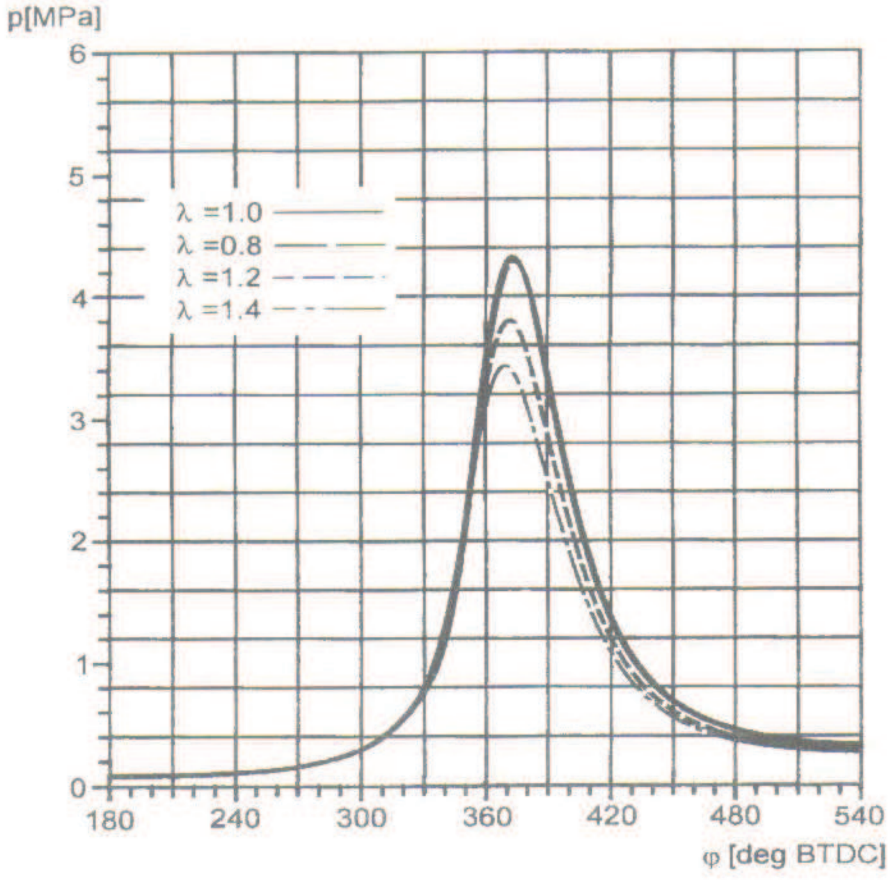

Fig. 10. Pressure in the cylinder vs. crank angle for different values of the coefficients of air excess for fuelling with gasoline. Ignition advance optimized for each λ on account on engine efficiency. $\eta_v=0.8$, $n=2500$ rpm

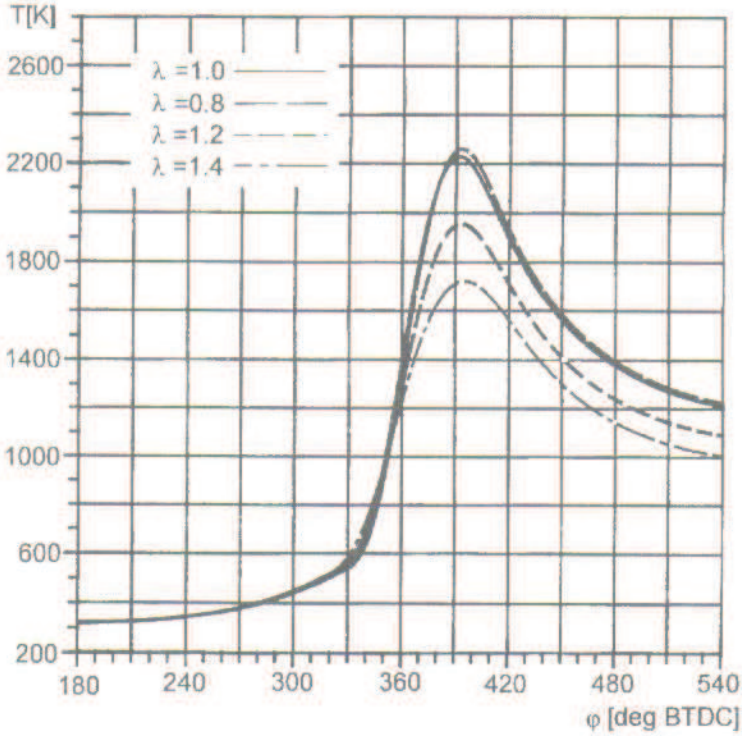

Fig. 11. Temperature of gases in the cylinder vs. crank angle for different values of coefficient of air excess. Conditions as in Fig. 10

Influence of engine operating parameters, i.e. of load (volumetric efficiency) and engine speed on pressure and temperature of gases in the cylinder are typical for SI engine.

4. Discussion of results

• Methanol burns quicker than gasoline [7] and fraction of burnt fuel x (Fig. 3) rises steeper for methanol than for gasoline. Also the pressure rises quickly and gets higher maximum values (Fig. 6 and Fig. 8). Due to that – among other reasons – enigne efficiency is higher for fuelling with methanol than with gasoline (Fig. 4 and Fig. 5), what confirms our earlier experiments with methanol engine [8]. Because of higher rate of burning, fuelling with methanol – in comparison with gasoline – demands smaller ignition advance, Fig. 6 and Fig. 8.

• Other main reason of higher efficiency for methanol fuelling in comparison with this for gasoline is smaller work of compression due to higher polytropic exponent k, Fig. 1.

• Next reason of higher efficiency for methanol fuelling in comparison with this for gasoline is higher value of molar conversion factor (defined as the ratio number of moles of products to number of moles of substrates) during combustion, resulting in higher pressure during expansion [7], that may be seen in Fig. 1.

• The influence of ignition timing on pressure and temperature inside the cylinder is in agreement with other published data, e.g. [3] and our yet not published experimental data. Also the influence of mixture strength on above mentioned parameters is correct and is in agreement with experimental data.

• The influence of mixture strength on engine overall efficiency is in agreement with experiments: for $\lambda < 1$ efficiency increases with λ. According to [9], decrease of efficiency with increase of λ for the engine begins for $\lambda > 1.3$.

5. Conclusions

5.1. Conclusions regarding kind of fuel

- Fuelling with alcohols results in:
  - higher cylinder pressure,
  - higher cylinder temperature than for fuelling with gasoline.
- Maximum overall efficiency may be obtained for fuelling with methanol in a large range of air-fuel ratio.

5.2. Conclusions regarding simulation

- Worked out programme of simulation of combustion processes in SI engine, though very simple, is however enough adequate to evaluate the influence of:
  - kind of the fuel,
  - engine operating parameters,
  - engine performance parameters

  on pressure and temperature time history in engine cylinder and engine efficiency.
- The programme enables to estimate of engine performances for given operating conditions.
- Higher efficiency of methanol fuelled engine in comparison with gasoline fuelling, previously experimentally determined by one of the present authors [8], has been numerically validated.
- Because the simulation model is zero-dimensional, uniform temperature of gases, which is much lower than in the burnt gas, can not be responsible for emission of NO_x. So the model can not be used for computation of NO_x emission.

• The model may be improved by introduction of more accurate formulae, e.g. of coefficient of heat transfer, and by addition of the model of charge exchange process and charge motion within the cylinder.

Main symbols

B – universal gas constant,
L_o – stoichiometric air/fuel ratio,
Q_b – heat released in chemical reaction,

Q_w – heat transfered to walls,
p – pressure,
T – temperature,
c_p, c_v – molar specific by constant pressure and constant volume, respectively,
f – mass fraction,
i – enthalpy,
n – number of moles,
u – internal energy,
x – fraction of burnt fuel,
λ – air excess coefficient,
φ – crank angle,
μ_i – molecular mass of component i.

Subscripts main

i – number of a component,
w – wall.

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Komputerowa symulacja silnika o zapłonie iskrowym zasilanego z uwzględnieniem rodzaju paliwa

Streszczenie

W artykule autor zaprezentował wyniki symulacji komputerowej obiegu silnika o zapłonie iskrowym przy uwzględnieniu rodzaju paliwa, jakim zasilany jest silnik. Model umożliwia obserwację zmian zachodzących w cylindrze przy zasilaniu dwoma gatunkami benzyny (różniącymi się składem chemicznym) oraz alkoholami: etylowym i metylowym.

Do opisu zjawisk w cylindrze zastosowano model zerowymiarowy homogeniczny. Prędkość wypalania się świeżego ładunku opisano za pomocą równania Vibego. Ilość wydzielonego ciepła opisano za pomocą różnicy energii wewnętrznej czynnika roboczego w każdym kroku iteracyjnym. Przyjęto, że czynnik roboczy zachowuje się jak gaz półdoskonały. Do opisu zmian parametrów termodynamicznych składników czynnika roboczego posłużono się funkcjami wielomianowymi z członem wymiernym McBride'a. Uwzględniono ponadto wymianę ciepła poprzez ścianki cylindra i omywającą go ciecz chłodzącą oraz straty mechaniczne.

Danymi wejściowymi do modelu są następujące parametry: współczynnik napełnienia, prędkość obrotowa silnika, kąt zapłonu, rodzaj paliwa, współczynnik nadmiaru powietrza i inne mniej ważne parametry charakteryzujące silnik.

W wyniku obliczeń otrzymuje się przebiegi ciśnienia w cylindrze, temperaturę czynnika, bieżącą ilość moli, pracę użyteczną jednego cyklu (a z tego parametru moment obrotowy i moc silnika).

Pomimo prostego modelu zaobserwowano dobre odwzorowanie zjawisk zachodzących w cylindrze. Porównano wyniki obliczeń dla ww. paliw. Symulacja uwidoczniła wyraźne różnice pomiędzy przebiegiem ciśnienia i temperatury w cylindrze w zależności od rodzaju paliwa. Stwierdzono wyższą sprawność obiegu przy zasilaniu alkoholem metylowym i większą wrażliwość obu alkoholi na zmianę kąta zapłonu.