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SOME ASPECTS OF EXHAUST COMPOSITION FORMING IN GAS ENGINES

Summary. A rapid chemical equilibrium composition model was applied to calculate the main combustion products from gas spark-ignition engine. The kinetic concentration of oxides of nitrogen were evaluated on the basis of their equilibrium concentration. To validate model, experiments were carried out in a tree cylinder gas engine. Results for CO, CO₂, O₂, and NO emission show good agreements for varied air fuel ratio, engine speed, ignition timing and cylinder temperature.

WYBRANE ASPEKTY FORMOWANIA SIĘ SKŁADNIKÓW SPALIN SILNIKA GAZOWEGO

Streszczenie. W artykule przedstawiono wybrane wyniki symulacji procesu spalania mieszaniny powietrzno-gazowej w trójcylindrowym silniku gazowym o zapłonie iskrowym. Do symulacji wykorzystano model dwustrefowy. Symulacja procesu spalania przeprowadzona była w oparciu o charakterystyki przepływu ciepła pomiędzy strefami komory spalania i ściankami cylindra, które określono na podstawie wcześniejszych badań [1,2,3]. Wykazano wpływ zasadniczych parametrów regulacyjnych, a w szczególności współczynnika nadmiaru powietrza i kąta wyprzedzenia zapłonu na formowanie się produktów spalania.

1. INTRODUCTION

A single-zone, gas spark engine simulation has been developed for studies of engine performance and fuel economy. A dual-zone combustion model of dividing combustion chamber into unburned mixture and burned products zones. The first law of thermodynamics is applied to each zone. This paper describes the model and shows that predicted combustion products are in good agreement with experimental data under rated speed and load condition. Furthermore, the applicability of simulation for performance studies under range of speeds and loads is demonstrated. The main aim of this work is to predict the exhaust concentration of carbon monoxide and oxides of nitrogen, which are among the regulated pollutants emitted from internal combustion engines. Carbon dioxide is also an element of interest in this work, owing to growing concern about global warming.

2. TEST ENGINE AND INSTRUMENTATION

A Perkins AD 3.152G 3-cylinder 2,4 liter, spark engine was used in this work. The engine would be described as a low speed with two valve for cylinder and a centrally located spark plug. The engine was coupled to a 150 kW dynamometer. The dynamometer was operated at selected speeds and engine throttle condition. The data acquisition system included transient system and emissions monitoring equipment. The steady state data acquisition system was use for monitoring and recording engine speed, torque, cylinder pressure, air and gas flow rate, intake temperature, gas temperature, exhaust temperature, and coolant inlet and outlet temperature, spark timing and other useful parameters. The emissions monitoring equipment included CO, CO₂, NO/NO_x, O₂ and hydrocarbon analyzers.

3. DESCRIPTION OF DUAL-ZONE MODEL AND COMPUTATIONAL ALGORITHM

A number of modeling approaches have been proposed and tested with various degrees of success. Based on their potential for thermodynamic resolution of working mixture, model range from zero-dimensional, single-zone, multi-zone, to quasi-dimensional and to multi-dimensional models. Detailed analysis of all these models is proved necessity of further investigation. As a consequence of this investigation the objective of this paper is developing a quasi-dimensional, zonal model and implementing it into comprehensive simulation of spark engine. Mathematical modeling of phenomenon of combustion makes it possible not only to simplify and shorten research process, but also fast obtainment information about:

- temperature formation in time of conversion in combustion chamber,
- course of burning process of mixture,
- combustion products forming,
- course of heat transfer to the cylinder walls.



Fig. 1. Gas engine Perkins AD 3.152 G on test stand Rys. 1. Silnik gazowy AD 3.152 G na stanowisku badawczym

For described investigations two mathematical models were used:

- single-zone, which is based on balance of energy, it makes possible observation of setting phenomena in time of compressing and expanding [1],
- dual-zone, which defines course of heat release, based on actual cylinder pressure or on cylinder pressure course determined by the first model [2].

In second model thin front of flame divided combustion chamber onto two separated zones from themselves infinitely. Value of temperatures for every from zones they were homogeneous, and temperature of front of flame is even temperature of exhaust gases. Exhaust gases as products of combustion are equilibrium solution of ten components, CO_2 , CO, H_2O , NO, N₂, H, O, O₂, H₂ and OH. Heat losses in combustion chamber may be counted according to well knowing hypothesis, however in this paper hypothesis of Serafimov was used. This hypothesis with large exactitude reproduced course of heat transfer to the cylinder walls in studied engine, Perkins AD 3.152G.

In dual-zone model of combustion process courses of changes of pressure $p=f(\phi)$ and changes of volume $V_i=f(\phi)$ are used. Model is described by following equations:

- balance of energy of unburned zone

$$dQ = dU_u + dI_u + p^* dV_u + dQ_{wu}$$
⁽¹⁾

- balance of energy of flame front

$$dI_{u} = dI_{b} + dQ \tag{2}$$

- balance of energy of burned zone

$$dI_b = dU_b + p^* dV_{wb}$$
(3)

- thermal equation of state of zones

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

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

- equation of state of quantities and volumes of substance

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

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

- degree burning of mixtures

$$=G_{b}/G$$
(8)

- degree of release of chemical contain energy in fuel

x≃

$$y = x * [1 - W_{db} / W_{du}]$$

where:

Uu, Ub	 internal energy of mixtures and combustion products,
I _u , I _b	 – enthalpy of mixtures and combustion products,
T_u, T_b	- temperature of mixtures and burned zone,
V_u, V_b	- temporary volume of mixtures and burned zones,
р	– cylinder pressure,
0	- heat flow to zone of mixture from front of flame,

(9)

Qwu, Qwb	- heat flow to walls of combustion chamber from mixtures and flame
	zones,
Gu, Gb	- mass of substance of mixtures and exhaust gases on cycle,
G	– mass of load on cycle,
x	- degree burning of load,
У	- degree of release of chemical contain energy in fuel,
W _{du} , W _{db}	- fuel value of mixtures and unburned gases,
φ	- crank angle.
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Mixture and combustion gases are treated as semi ideal gases. For delimitation of molar parts components (I) of combustion gases were applied:

- Dalton's right

$$\mathbf{p}_{is} = (\mathbf{i})^* \mathbf{p} \tag{10}$$

- equation of balances of elements of carbon, hydrogen, oxygen and nitrogen

$$n_{Cf} = n_s^* [(CO_2) + (CO)]$$
(11)

$$n_{\rm Hf} + 2^*({\rm H_2O})^* \lambda^* n_{\rm amin} = n_{\rm s} [2^*({\rm H_2}) + 2^*({\rm H_2O}) + ({\rm OH}) + ({\rm H})$$
(12)

$$n_{Of} + [2^{*}(O_{2})_{a} + (H_{2}O)_{a}]^{*} \lambda^{*} n_{amin} = n_{s}^{*} [(CO) + 2^{*}(CO_{2}) + 2^{*}(O_{2}) + (H_{2}O) + (O) + (NO)]$$
(13)

$$n_{Nf} + 2^{*}(N_{2})_{a} * \lambda * n_{amin} = n_{s} * [2^{*}(N_{2}) + (NO)]$$
(14)

- equation catfishes of parts

$$(CO_2)+(CO)+(O_2)+(H_2)+(H_2O)+(OH)+(H)+(O)+(NO)+(N_2) = 1$$
(15)

- equations of defining equilibrium constant K of chooses reaction:

$$CO_2 \leftrightarrow CO + \frac{1}{2}O_2 \qquad K_1 = \frac{(CO)^*(O_2)^{\frac{1}{2}}}{(CO_2)} * p^{\frac{1}{2}}$$
(16)

$$H_2 O \leftrightarrow H_2 + \frac{1}{2}O_2 \qquad K_2 = \frac{(H_2)^*(O_2)^{\frac{1}{2}}}{(H_2 O)^*} * p^{\frac{1}{2}}$$
 (17)

$$H_2 O \leftrightarrow OH + \frac{1}{2} H_2 \qquad K_3 = \frac{(OH)^* (H_2)^{\frac{1}{2}}}{(H_2 O)} * p^{\frac{1}{2}}$$
(18)

$$\frac{1}{2}H_2 \leftrightarrow H \qquad \qquad K_4 = \frac{(H)}{H_2} * P^{\frac{1}{2}}$$
(19)

$$\frac{1}{2}O \leftrightarrow O \qquad K_{5} = \frac{(O)}{(O_{5})^{\frac{1}{2}}} * p^{\frac{1}{2}}$$
(20)

$$\frac{1}{2}N_{2} + \frac{1}{2}O_{2} \leftrightarrow NO \qquad K_{6} = \frac{(NO)}{(N_{2})^{\frac{1}{2}} * (O_{2})^{\frac{1}{2}}}$$
(21)

In these equations:

 $\begin{array}{ll} n_{Cf}, n_{Hf}, n_{Of}, n_{Nf} - \mbox{quantity of kilomole of element C, H, CO, N in fuel onto individual fuels,} \\ n_{a} & - \mbox{quantity of kilomole of moist fumes onto individual fuels,} \\ n_{amin} & - \mbox{this theoretical demand kilomole of air to burning of individual fuels,} \\ \lambda & - \mbox{relation of excess of air in load,} \\ p_{is} & - \mbox{this partial pressure and - this component of fumes.} \end{array}$

Dissolving simultaneously introduced above equation values of temperatures of zones of mixture were marked ere and fumes T_b as well as chemical warehouse of fumes in function of angle of turn of crank rampart. Calculations were completed in accordance with introduced algorithm on drawing 2.



Fig. 2. Algorithm of solving dual-zone model of combustion Rys. 2. Algorytm zastosowany do rozwiązania równań

4. RESULTS OF CALCULATIONS AND DISCUSSION

Courses of: gases average temperature T_{av-max} , maximum temperature in burned zone T_{bmax} , and exhaust gases temperature (counted- T_{bg} and measured- T_{eg}) in dependence from coefficient λ are presented on drawings 3 and 4.

From exploitation and ecological point of view it is very important to assurance of such conditions of work, which do not cause excessive thermal load as well as they do not cause excessive emission of toxic components in combustion gases. Hence, increasing coefficient λ , the lean operation decreasing as well average combustion temperature as exhaust gases. The difference between calculated and measured gas temperature in exhaust manifolds cased to well-known circumstance. The measuring by the thermocouple temperature of pulsing flow gives overestimated results. The error of this measurement increases when the relation between pulse pressure difference and average value of pressure increases. The changes of temperatures in combustion chamber, which were got as a result of calculations, explain also, that increase of engine load influence onto stabilisation of thermal load of combustion chamber. Suitable changes of regulate parameters such as spark timing and mixture composition give a possibility of decreasing temperature inside cylinder.

Composition of combustion gases formed during combustion process depends on value of cylinder pressures and values of temperature in burned zone. The example of course of formation of 10 components in combustion gases as a function of crank angle, for one of engine loads is presented on drawing 5.



- Fig. 3. Characteristic temperatures of combustion in dependence of air excess ratio. Throttle opening ratio=25%
- Rys. 3. Zależność temperatur spalania od współczynnika nadmiaru powietrza, dla 25% otwarcia przepustnicy



- Fig. 4. Characteristic temperatures of combustion in dependence of air excess ratio. Throttle opening ratio=50%
- Rys. 4. Zależność temperatur spalania od współczynnika nadmiaru powietrza, dla 50% otwarcia przepustnicy

However on drawing 6 results of calculations of combustion gases for choose loads of engine were introduced in dependence from air-fuel ratio mixture. On this drawing were put also results, which were got during stand engine tests. The biggest changes of course of combustion depend on mixture changes. Mixture burning ratio decreases violently when air fuel ratio exceeds stoichiometric value, $\lambda > 1$. For tested engine fuelled by LPG, essential changes set yet in range of changes of air excess coefficient in range from 1 to 1,1. A content of CO is decreased tenfold, similar character of changes was observed for HC.

In range of lean mixtures, that is for $\lambda > 1$ high content O₂ was affirmed and NO, however in range of rich mixtures it was observed increase, HC and CO. results which has been got define best value of coefficient λ for studied engine. For this value of coefficient content CO₂ is the highest. Results in model calculations are lower about 0,8% compare with these, which were got in stand engine tests.



- Fig. 5. An example of forming 10 components of exhaust gases during combustion, throttle opening ratio=50%, rpm 1750, air excess ratio 1,08 and ignition advance 5⁰
- Rys. 5. Przykład formowania się 10 składników w spalinach silnika, dla obciążenia silnika 50%, n=1750 obr/min, λ=1,08 i kąta wyprzedzenia zapłonu 5°



- Fig. 6. Exhaust gases composition in dependence on air excess ratio, for throttle opening ratio 50%, rpm 1750, ignition advance 12°
- Rys. 6. Produkty spalania w zależności od współczynnika nadmiaru powietrza, obciążenie 50%, n=1750 obr/min, kąt wyprzedzenia zapłonu 12°

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Abstract

A dual zone model has been applied to simulate combustion of fuel-air mixture in a three-cylinder spark ignition internal combustion engine, focusing on the predictions of emissions in good agreement with experimental data. Model presented in this paper gives possibilities of leading further investigation based on obtained characteristics of heat flow between combustion chamber zones and cylinder walls. The simulation of combustion process shows changes of forming composites of exhaust gases as a result of regulation and engine major parameters.

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