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# NUMERICAL ANALYSIS OF SOME PARAMETERS OF GAS ENGINE

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**Summary**. The paper presents the results of the modelling of gas engine thermal cycle using AVL FIRE and KIVA 3V software. There are described three combustion models used in the above-mentioned software. KIVA and FIRE are used in the Institute of Internal Combustion Engines and Control Engineering for an analysis of thermal cycle of internal combustion (IC) engines. FIRE gives many possibilities with many combustion models, but they require verification. Comparison of modelling results of thermal cycle of IC engine is presented in the paper. All the used combustion models are dependent on turbulence of flow field before ignition. Pressure, temperature, heat transfer and turbulence parameters variations in the function of crank angle as well as spatial distribution of the above-mentioned quantities at the selected crank angles were determined.

**Key words**: internal combustion engine, thermal cycle, modelling, combustion

## INTRODUCTION

The numerical simulations with advanced computer programs give possibilities for very complicated processes research conduct. In 2009 the Institute of Internal Combustion Engines and Control Engineering began University Partnership Program with AVL Company concerning the modelling of thermal cycle of IC engines using FIRE software. Connection of advanced programs with contemporary computers give a chance to model turbulent flow and heat processes with combustion, fuel injection, heat transfer, toxic components of exhaust gas and soot. In spite of this, models are still incomplete, which requires many values taken for the experiment. Moreover, numerical simulations allow the researchers to observe spatial distribution of individual parameters. This makes it easier to understand very complicated processes. Mathematical modelling gives possibility to optimize the shape of an intake manifold, an exhaust or a combustion chamber. This method is an essential method in design and optimization. The paper presents results of combustion process modelling in spark ignition test engine Deutz 1650 $cm^3$. The modelling was carried out using three-dimensional CFD: AVL FIRE and KIVA-3V.

## AVL FIRE PROGRAME CHARACTERISTIC

The AVL FIRE software belongs to contemporary programs which are used for modelling of thermal cycle of internal combustion engines. FIRE allows for the modelling of flow and thermal processes occurence in the intake manifold, in combustion chamber of IC engine and exhaust pipe with a catalyst and a particulate filter. This programme enables the calculation of transport phenomena, mixing, ignition and turbulent combustion in internal combustion engine. Homogeneous and inhomogeneous combustion mixtures in spark ignition and compression ignition engine can be modelled using this software, as well. Kinetics of chemical reactions phenomena is described by combustion models which take oxidation processes in high temperature into consideration. Several models apply to auto ignition processes. AVL FIRE allows for the modelling of knock process which occurs in combustion chamber of IC engine. In five models, with different complication levels, an influence of turbulence intensity on combustion rate is considered. The choice depends on the modelled object or calculation possibilities. The user can use several combustion models: Eddy Breakup Model, Turbulent Flame Speer Closure Model, Cohorent Flame Model, PDF Model, NO formation models: Extendend Zeldovich Models, Heywood Models, soot formation and oxidation models: Lund Flamelet, Frolov Kinetic, Kennedy/Hiroyasu/Magnussen, turbulence models: k-epsilon, k-zeta-f, laminar, LES, ignition models: Diesel, Diesel Multiple Ignition Location, HCCI, Knock (Shell Model), Knock (Shell Model with temperature coupling), AnB Knock, Empirical Knock Model, Diesel ignited gas engine, complex fuel spray models and others. There is reach library of fuels like petrol, diesel and hydrogen or DME. This program allows for the building of three-dimensional computational greed, characterized by boundary conditions of surfaces and initial conditions of simulation. The postprocessor gives a possibility for visualization of results. AVL FIRE version 2009 include FIRE ESE Diesel module which was designed for modelling diesel combustion chambers. Injector is modelled as an element which takes place inside the combustion chamber. The shape of combustion chamber and tip of injector can be freely shaped. The project of combustion chamber can be imported from other CAD programs. FIRE allows importing meshes from many specialist programs. In the Institute of Internal Combustion Engines and Control Engineering computational mesh is generated by ICEM CFD software. FIRE allows to take boundary layer into consideration.

## COMBUSTION MODELS IN AVL FIRE

Two models were taken into account: Eddy Breakup Model (EBM) and Turbulent Flame Speed Closure Model (TFSCM) [3]. In both models the oxidation processes of a fuel with air is determined by turbulent processes which occurs in combustion chamber. Combustion process is described by a single step irreversible reaction:

$$1kg\{C_nH_mO_k\} + Skg\{a_1O_2 + a_2N_2\} \Rightarrow (1+S)kg\{a_3CO_2 + a_4H_2O + (1-a_3-a_4)N_2\}, \quad (1)$$

where:

$a_1$, $a_2$, $a_3$, $a_4$, S – dimensionless coefficients for reactions,

## EDDY BREAKUP MODEL (EBM)

The Eddy Breakup Model (EBM) [3] represents models which are based on turbulent mixing mechanism. This type was described by Magnussen, Hjertegar and Spalding. This model assumes that a turbulent flame, fuel and oxygen are situated in the same eddies which are separated from eddies containing hot combustion products.

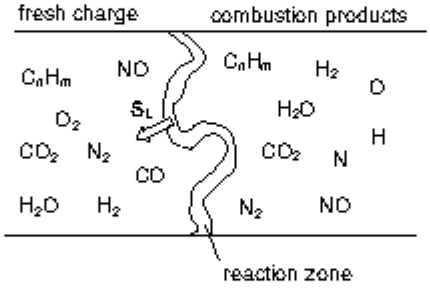



Fig. 1. Idea of turbulent combustion model

In the worked out by Magnusen model the results mainly depend on turbulent field of fresh charge parameters. The rate of combustion is determined by the rate of intermixing on the smallest scales of eddies containing fuel and oxygen. This is determined by the rate of dissipation of eddies. The rate of chemical reactions depends on an initial kinetic energy and turbulent length scale as well. The time scales of the chemical reactions are very short compared with the scales which determine turbulent transport processes. The mean rate of the chemical reaction can be described as:

$$\omega_{x_i} = -\frac{C_{x_i}}{\tau_R}\bar{\rho}\min\left(\bar{y}_{x_i}, \frac{\bar{y}_{O_2}}{S}, \frac{C_{Pr}\bar{y}_{Pr}}{1+S}\right). \tag{2}$$

The first two quantities of the "minimum" operator determine whether the reactants are present in adequate quantity for a chemical reaction to occur. The third of them determines reaction probability. This ensures that the flame is not spread without hot products. $C_{fu}$ and $C_{Pr}$ are empirical coefficients, $\tau_R$ is the turbulent mixing time scale for reaction. Coefficient $C_{fu}$ depends on turbulence and fuel parameters. This parameter requires adjustment with respect to experimental combustion data from the real engine. The general assumption is that the rate of combustion processes depends on the intermixing rate occuring in molecular scales, in eddies containing reactants and hot products and eddies formed as a result of dissipation process. The advantage of this model is its simplicity, which does not involve knowledge of many parameters of chemical reactions. In this model, worked out by Magnusen, the results mainly depend on turbulent field of fresh charge parameters like initial turbulent kinetic energy and turbulent time and length scales.

## TURBULENT FLAME SPEED CLOSURE MODEL (TFSCM)

The Turbulent Flame Speed Closure Model is destined for modelling combustion processes of homogeneous and inhomogeneous mixtures in spark ignition engine. The essence of this model is the determination of the rate of chemical reactions depending on fresh charge turbulence parameters in the cylinder of internal combustion engine. The turbulence intensity and turbulence scales of charge have significant impact on combustion process. These parameters have influence on fire

structure like the flame thickness and flame spread. The rate of chemical reaction is described by two mechanisms: first - auto ignition model (AI) and second - flame propagation scheme (FP).

The first one is described by Arrhenius equation. In the second mechanism the flame propagation mainly depends on the turbulent flame speed. Depending on conditions one of these mechanisms is the dominant one. The fuel reaction rate can be described by operator:

$$\omega_{fc} = \max\left(Auto-ign\ \omega_{AI}, Flame\mathbf{P}ropagation\ \omega_{FP}\right). \tag{3}$$

The first mechanism was constructed for combustion air factor 0.5 to 0.65 and pressure from 0.3 to 12 MPa. The rate of auto ignition reaction is described by:

$$\omega_{AI} = a_1 \rho^{a_2} y_{fuel}^{a_3} y_{O_2}^{a_4} T^{a_5} \exp\left(-\frac{T_a}{T}\right), \tag{4}$$

where:

$a_1 \ldots a_5$ - empirical coefficients,
$T_a$ - activation temperature,
$T$ - temperature.

In the second mechanism, the reaction rate $\omega_{FP}$ is described by gas density, turbulent combustion speed $S_t$ and gradient of mass fraction $\nabla y_{fuel}$.

$$\omega_{FU} = \rho S_T \nabla y_{fuel}. \tag{5}$$

Initially this model had been worked out for homogenous premixed combustion mixtures, next was adapted to inhomogeneous charges. Previous relationship which described reaction rate $\omega_{FP}$ was written as the product of the gas density, fuel mass fraction gradient and the turbulent burning velocity.

$$\omega_{FP} = \rho S_T \nabla cf_{st}. \tag{6}$$

This approach was described for homogeneous premixed combustion mixtures and near-wall treatment of the reaction rate. Small eddies of fresh charge and the other motions of fluid cause increase the flame front. The flame surface increase cause increase of combustion rate of air-fuel mixture. The high turbulence level which causes the high flame propagation rate in internal combustion engine can be achieved by squish effect and the suitable shape of the combustion chamber.

## COMBUSTION MODEL IN KIVA 3V

Numerical researches were conducted using also KIVA-3V software. The engine work cycle model in the code is based on the system of mass, momentum and energy conservation equations describing three dimensional, unsteady flow fields with chemical reactions (combustion). The code solves three-dimensional Navier-Stokes equation for the mixture of compressible liquids, which enables taking into account creation and development of shock wave in gas. Periodic boundary conditions and walls (with turbulent wall law, free slide and without slide, with adiabatic wall and with diversified temperature distribution on the wall) are used as boundary conditions in the KIVA-3V code. Three turbulence models are implemented: *k-ε, RNG k-ε* and *SGS (Sub-Grid Scale)*.

The combustion submodel consists of four kinetic and six equilibrium reactions. The kinetic reactions are: one global reaction (oxidation of hydrocarbon fuel $C_nH_m$) with extended Zeldovich

mechanisms for $NO_x$ formation. The rate of equilibrium reaction does not depend on time and depends only on temperature.

$$C_nH_m + O_2 \overset{k}{\Rightarrow} CO_2 + H_2O \tag{7}$$
$$O + N_2 \Leftrightarrow NO + N \tag{8}$$
$$N + O_2 \Leftrightarrow NO + O \tag{9}$$
$$N + OH \Leftrightarrow NO + H \tag{10}$$

The equilibrium reactions are:

$$H_2 \Leftrightarrow 2H \tag{11}$$
$$O_2 \Leftrightarrow 2O \tag{12}$$
$$N_2 \Leftrightarrow 2N \tag{13}$$
$$O_2 + H_2 \Leftrightarrow 2OH \tag{14}$$
$$O_2 + 2H_2O \Leftrightarrow 4OH \tag{15}$$
$$O_2 + 2CO \Leftrightarrow 2CO_2 \tag{16}$$

The kinetic reaction proceeds at the rate of $\dot{\omega}_r$ given by:

$$\dot{\omega}_r = k_r \prod_j \left[\frac{\rho_j}{M_j}\right]^{a_j} = k_r [C_nH_m]^{a_1} [O_2]^{a_2} \tag{17}$$

where:

$k_r$- rate coefficient for reaction,
$\rho_i$- mass density of species i,
$M_i$- molecular weight of species i,
$a_1, a_2$- integer stoichiometric coefficients for reaction.

Rate coefficients for reaction are assumed to be of a generalized Arrhenius form:

$$k_r = A_r T^{r} \exp\left(-E_r / T\right) \tag{18}$$

where:

$A_r$- constant,
$E_r$- activation energy,
$T$- temperature.

## RESEARCH OBJECT

The research object was a spark ignition engine powered by gas fuel. This is test engine which was adapted from two cylinders compression ignition engine DEUTZ. The result of the reconstruction was adaptation of this engine to combustion of methane and decreased compression ratio to 8.

Table 1. Main engine parameters

| | |
|---|---|
| Compression ratio | 8 |
| Stroke | 105 mm |
| Cylinder diameter | 100 mm |
| Engine cubic capacity | 825 $cm^3$ |
| Number of cylinders | 2 |
| Direction of cylinders | vertical |
| Length of connecting-rod | 136 mm |
| Rotational speed | 1500 rotation/min |

Figure 2 shows cross-section of cylinder of the test engine with asymmetrically placed sparking plug.

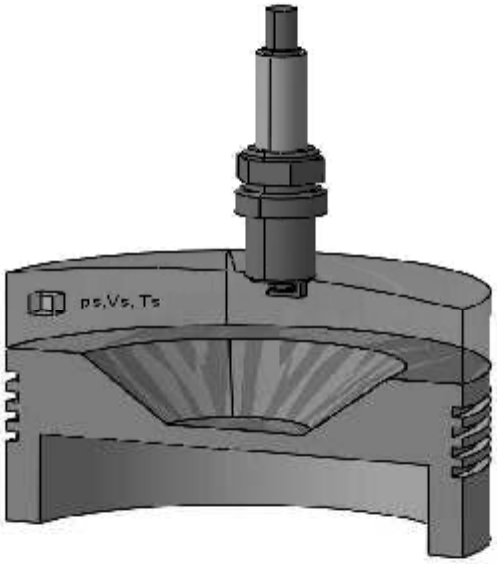



Fig. 2. Combustion chamber of the modeled engine [7]

## MODELLING OF THERMAL CYCLE OF TEST ENGINE

Modelling in AVL FIRE and KIVA 3V software was conducted for gas fuel – methane, for these same boundary and initial conditions. In both cases $k - \varepsilon$ turbulence model was used. The computational mesh of combustion chamber of the test engine in both cases was made of this same number of cells and nodes.

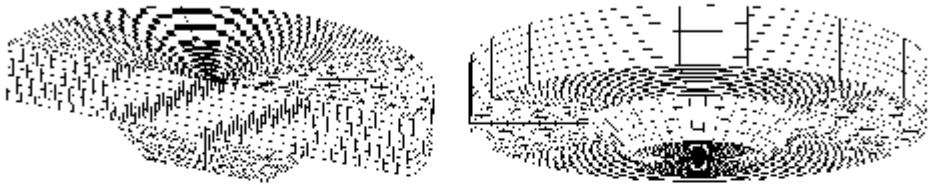


Fig. 3. Geometric mesh of combustion chamber at TDC

The model of fuel-air mixture ignition requires an ignition crank angle occurrence, volume of ignition area and its location inside combustion chamber. There is a possibility to model multi spark plug ignition and allow for the modelling combustion knock process.

Calculation started in BDC at the beginning of compression stroke for these same starting conditions and finished at 180 degree after TDC. Calculations were conducted for combustion air factor equal to 1.0 and ignition crank angle equal to 10 degree before TDC.

Table 2. Chosen input parameters of the modelled process

| | |
|---|---|
| Ignition timing | 10° before TDC |
| Combustion air factor | 1.0 |
| Initial temperature | 293 K |
| Initial pressure | 0.9 bar |
| fuel | $CH_4$ |
| Turbulence kinetic energy (180° before BDC) | 0,1 $J/m^3$ |
| Turbulence length scale (180° before BDC) | 1,12 cm |

## RESULTS OF CALCULATIONS

A number of characteristic quantities of the combustion process in the test engine were obtained as a result of numerical analysis. The chosen quantities of courses are presented in the figures below. Pressure courses in the analyzed engine are presented in Figure 4. In both cases for FIRE and KIVA 3V the compression pressure achieved the same value. Results of modeling in KIVA 3V code and AVL FIRE using Eddy Breakup model achieved almost the same course. TFSC model used in AVL FIRE caused bigger differences in the maximum peak of pressures. Combustion process in this case proceeded relatively slowly.

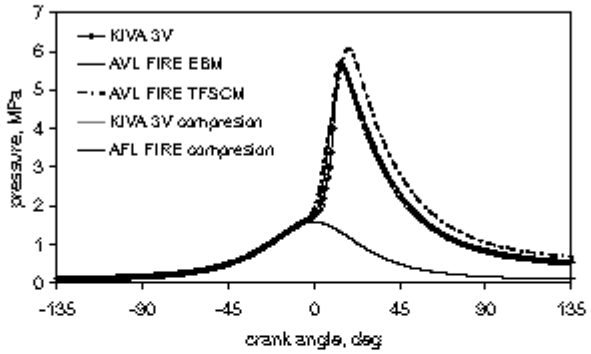



Fig. 4. Pressure courses in the analysed engine

The heat release and heat release rate courses are presented in Figure 5. TFSC model in analysed case gave the biggest heat release. Heat release in this case was characterised by long time duration. Results obtained from KIVA 3V code were characterised by smaller heat release but heat release rate occured faster.

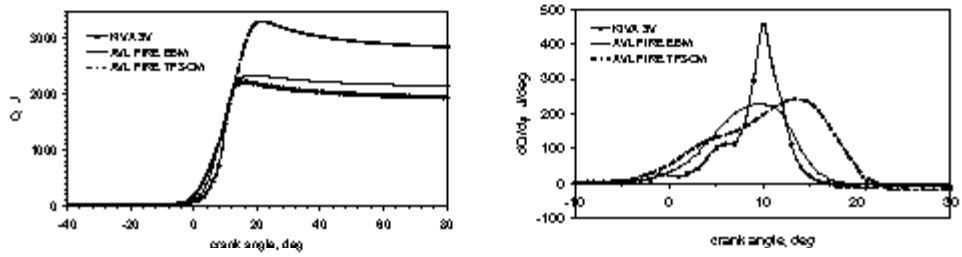



Fig. 5. Heat release and heat release rate

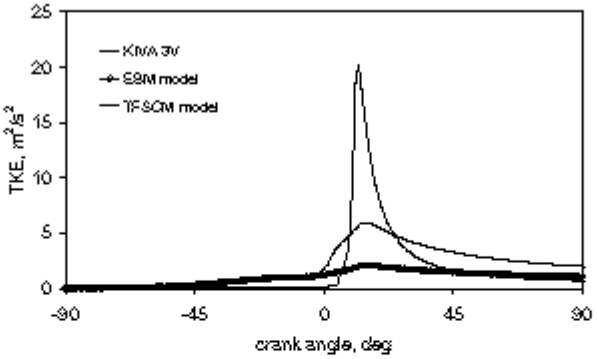



Fig. 6. Turbulent kinetic energy

The maximum value of turbulent kinetic energy was achieved during flame spread. The maximum value of turbulent kinetic energy obtained from KIVA 3V code has by several times higher level then the one obtained from other models.

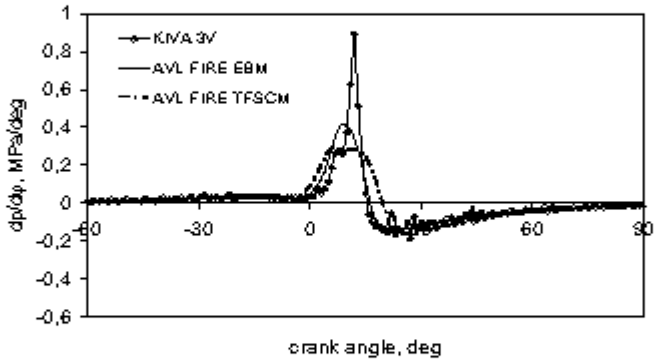
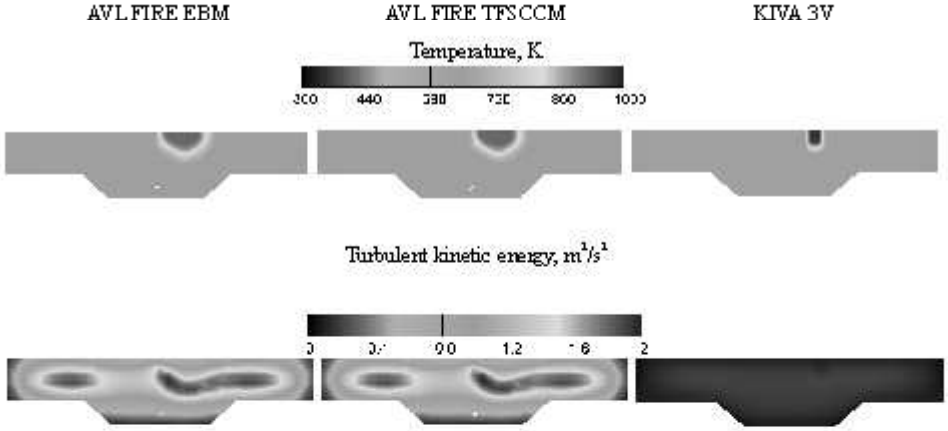



Fig. 7. Pressure growth speed courses in the function of crank angle

KIVA 3V code gave in this case the highest increase of pressure which in consequence had an influence on other parameters of the thermal cycle. Maximum dp/dφ gained the value of 0,9 MPa/deg in KIVA 3V code and the smallest increase in pressure was obtained from TFSC model 0,3 MPa/deg. Spatial distribution of temperature and turbulent kinetic energy in combustion chamber of the test engine are presented below:

**8 deg before TDC**



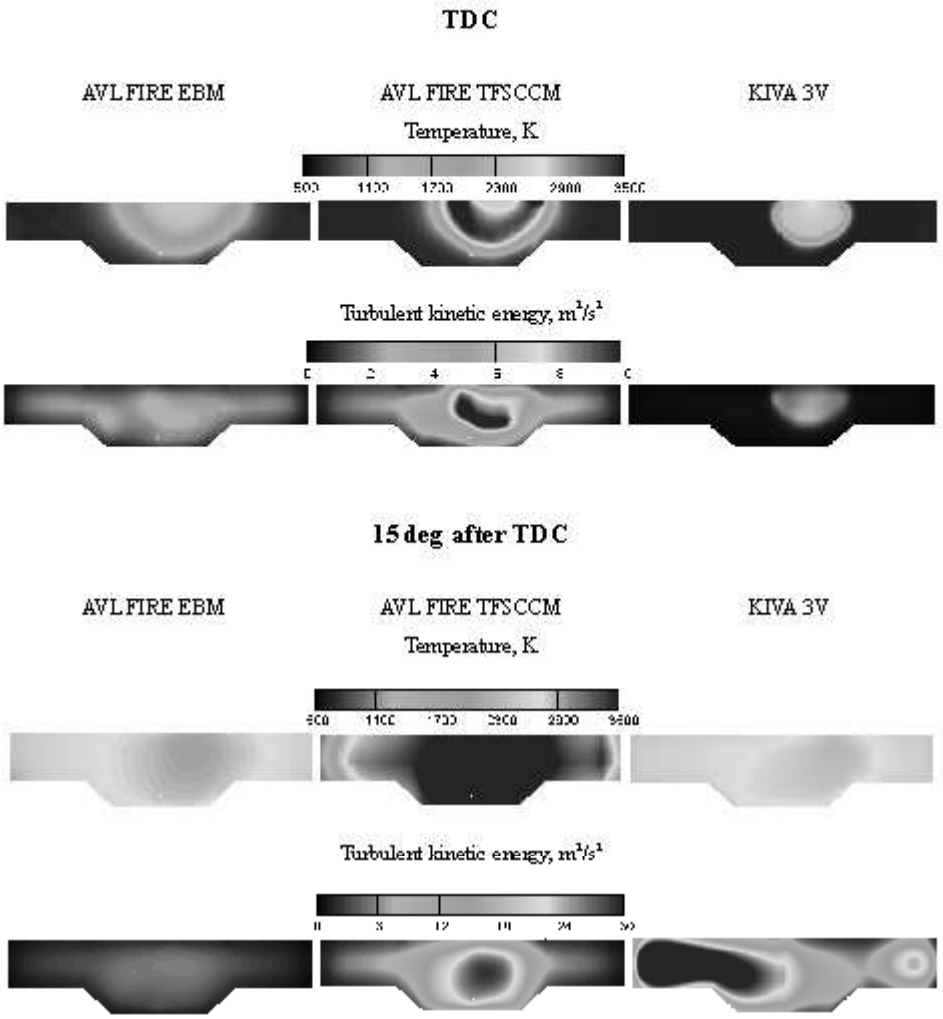



Fig. 8. Spatial distribution of temperature and turbulent kinetic energy in the selected crank angles

## CONCLUSIONS

The paper presents results of modelling gas engine thermal cycle using AVL FIRE and KIVA 3V software. There are described three combustion models used in the software. KIVA and FIRE software are used in the Institute of Internal Combustion Engines and Control Engineering for an analysis of the thermal cycle of IC engines. Comparison of modelling results of the thermal cycle of IC engine is presented in the paper. All the used combustion models are dependent on turbulence of flow field before ignition. FIRE software gives many possibilities with many combustion models, but they require verification. Pressure, temperature, heat transfer and turbulence parameters varia-

tions in the function of crank angle as well as spatial distribution of the above-mentioned quantities at the selected crank angles were determined.

This same initial and boundary conditions were assumed in all the analysed cases. Results are different with respect to values and courses. Unfortunately, this article did not include results of experiment. Comparison of modelling and experimental results will be presented in the next paper.

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## ANALIZA NUMERYCZNA WYBRANYCH PARAMETRÓW SILNIKA GAZOWEGO

**Streszczenie:** Modelowanie numeryczne z wykorzystaniem coraz bardziej zaawansowanych programów komputerowych umożliwia relatywnie niskim kosztem prowadzić badania bardzo skomplikowanych procesów. Instytut Maszyn Tłokowych i Techniki Sterowania od 2009 roku, w ramach University Partnership Program z firmą AVL, do modelowania obiegu cieplnego silnika tłokowego wykorzystuje program AVL FIRE. Połączenie tak

zaawansowanych programów komputerowych z możliwościami obliczeniowymi współczesnych komputerów daje możliwości modelowania turbulentnych procesów cieplno-przepływowych ze spalaniem, wtryskiem paliwa, wymianą ciepła oraz mechanizmami tworzenia się toksycznych składników spalin i sadzy. Mimo to, są to ciągle modele niekompletne, wymagające szeregu wartości wielkości wejściowych zaczerpniętych z eksperymentu. Modelowanie w układzie 3D daje dodatkowo możliwość obserwacji poszczególnych parametrów w czasoprzestrzeni, co znacznie ułatwia poznanie często bardzo złożonych zjawisk. Modelowanie takie daje możliwość optymalizacji kształtu układu dolotowego, wydechowego czy komory spalania. Jest to metoda nieodzowna w procesie projektowania i optymalizacji.

W prezentowanej pracy przedstawiono wyniki modelowania procesu spalania w badawczym silniku o zapłonie iskrowym Deutz 1650 $cm^3$. Modelowanie przeprowadzono przy użyciu wykorzystywanych w IMTiTS Politechniki Częstochowskiej, nowoczesnych programów do modelowania trójwymiarowego CFD: AVL FIRE oraz KIVA-3V.

**Słowa kluczowe:** komora spalania, cykl termiczny, modelowanie, spalanie