# SIMULATION OF EXHAUST GASES COMPONENTS FORMATION IN ENGINE WORKING WITH COMBUSTION INITIATION FROM IGNITION DOSE OF FUEL

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#### Abstract

The paper deals with problems of model analysis of the process of exhaust gases components formation in internal combustion engine working with combustion initiation from ignition dose of fuel injected directly into the working space. In result of scientific-research works carried out in the Chair of Internal Combustion Engines of Cracow University of Technology on the basis of a four stroke engine a driving unit was elaborated which may work both with spark ignition and combustion initiation from a ignition dose of fuel. Application of two combustion systems in engine aimed at combining the advantages of spark ignition with compression ignition driving units. Such an engine is characterized by fuel consumption comparable with that gained by compression ignition engines, whereas, the exhaust gases composition is similar to that occurring in up-to-date spark ignition engines. Similar assumption concern the Homogenous Charge Compression Ignition – HCCI system which seems to be a future solution of internal combustion engines, nevertheless, up till now, in spite of intensive works in many countries all over the world, one did not succeed to control the combustion process in a large range of rotational speeds and loads what would give the possibility of using it in traction application. The solution proposed in the patent application by Prof. B. Sendyka is not burdened with this drawback since the moment of occurrence of volumetric ignition of the formed mixture in the process of filling is tightly connected with the moment of fuel dose injection. In result of simulative studies carried out by use of KIVA-3V software on the discussed solution it was stated that the process of exhaust gases toxic components formation in engine working in the mode of ignition from pilot dose does not depart in generally form from that which occurs at work with spark ignition.

Keywords: modelling, simulation, spark ignition, compression ignition, exhaust gases emission

#### 1. Introduction

The article deals with topics of scientific - research works which concern formation of combustion products in combustion engine in which ignition is realized by use of fuel dose injection applied directly into the combustion chamber. Analysis of results of the carried out simulation works was to determine how far the assumption that the composition of exhaust gases of engine working in mode of combustion initiated by pilot dose injection does not depart in principally from exhaust gases composition of engine working with spark ignition.

#### 2. Simulation studies

Numerical analysis of the process of formation of exhaust gases was carried out by use of KIVA-3V software. The studies were to determine the character of formation of exhaust gases components and visualization of distribution of their mass fraction in the cylinder of engine working with combustion initiation from dose whose quantity was defined as 5% of total fuel mass consumed by engine. The rest of fuel was injected into the engine intake manifold. Direct injection of the ignition dose started at 38 °CA before TDC.

Simulation works carried out in KIVA-3V software for the needs of this elaboration concerned mainly:

- numerical simulation of work cycle of engine working with combustion with combustion initiation from injection of fuel ignition dose,
- elaboration of diagrams of traces of engine exhaust gases parameters on the basis of numerical calculation results,
- visualisation of the process of formation of chemical components of exhaust gases

One of the cylinders of 2SZ-FE Toyota engine was the object of simulation investigations. The rotational speed was established on the level of 2000 RPM. The numerical grid of the cylinder of the engine was constructed by use of pre-processor of the KIVA-3V tool. The grid was irregularly concentrated. Densification of layers in the TDC region was applied in order to improve calculation accuracy. The engine cylinders were numerically approximated respectively in axis X - 38, in axis Y - 34, and in axis Z - 36 computational cells. The proper computational process was preceded by preliminary simulations in order to establish correctness of the computational process.

Figure 1 presents cross-section of valves of the computational grid of the engine on the basis of piston position 66° CA after TDC.

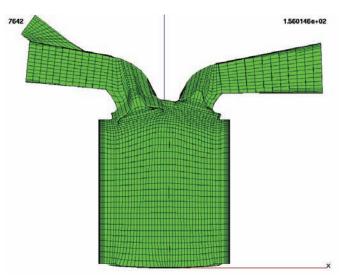


Fig. 1. Computational grid of the 2SZ-FE engine

Initial and boundary data adopted in simulation investigations are listed below:	
Fuel mass dosed to the intake manifold	0.02085g
Mass of the ignition dose of fuel	0.001125 g
Rotational speed	2000 RPM
Angle of start of fuel injection into the intake manifold	360 ° CA before TDC
Angle of start of ignition dose injection	38 ° CA before TDC
Absolute pressure in the exhaust port	0.1 MPa
Absolute Pressure in the intake port	0.13 MPa
Position of injector with respect to cylinder Z-axis	68 °
Model of turbulence	k-ε
Number of chemical compounds	12

# 3. Formation of chemical compounds during combustion

The KIVA-3V software disposes of possibility of presentation of mass fraction of chemical compounds in the cylinder, in the intake and exhaust, as well as distribution of these quantities in the volume of the considered space [2].

The process of carbon dioxide formation during combustion was illustrated by the diagram in Fig. 2.

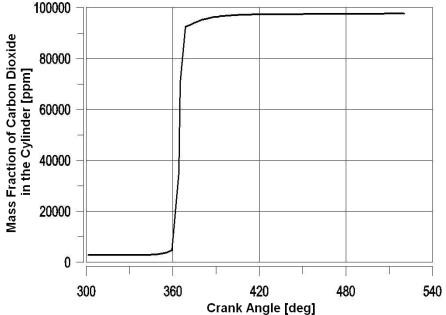


Fig. 2. Change of mass fraction of carbon dioxide in cylinder in function of crank angle

Figure 3 presents mass fraction of carbon monoxide in cylinder in function of crank angle.

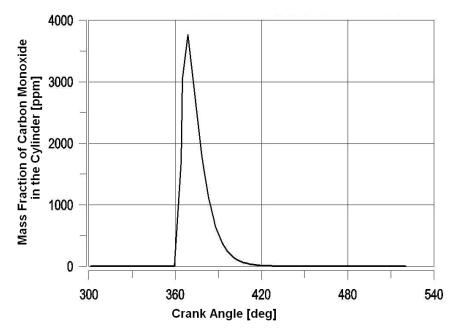


Fig. 3. Change of mass fraction of carbon monoxide in the cylinder in function of crank angle

Basing upon analysis of traces presented in Fig. 2 and 3 it was found that in the period of fast burn both carbon monoxide as well as carbon dioxide is formed in the cylinder, whereas, during the afterburning phase the harmful carbon monoxide undergoes oxidation to dioxide [4].

Figure 4 shows the traces of nitric oxide formation in the cylinder of engine working with combustion initiated from an ignition dose of fuel.

During fast burning intensive formation of nitric oxide takes place, whereas, a drop of NO concentration in the consequent phase of the process is connected with oxidation of this compound at lowered temperature to NO<sub>2</sub>.

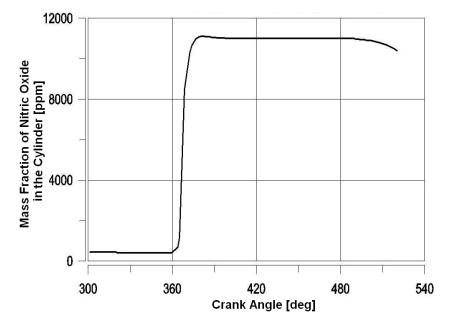


Fig. 4. Traces of mass fraction of nitric oxide NO in cylinder charge of function of crank angle

#### 4. Three-dimensional visualisation of distribution of exhaust gases components

The KIVA-3V software permits to a three-dimensional visualisation of images presenting mass fraction of components of exhaust gases in function of crank angle [1].

Figure 5 presents distribution of mass fraction of hydroxyl radicals in the engine cylinder at piston position 23° CA after TDC.

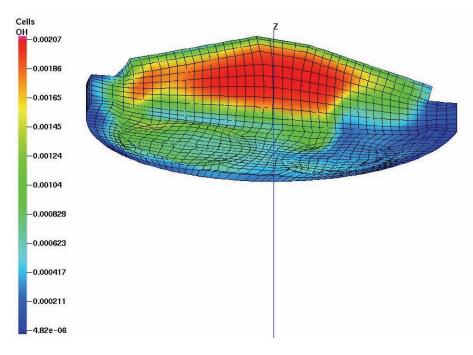


Fig. 5. Distribution of mass fraction of hydroxyl radicals OH in cylinder at piston position 23° CA after TDC

Distribution of OH radicals in combustion chamber is of irregular character resulting from charge movement in the cylinder.

Figure 6 shows distribution of mass fraction of carbon monoxide in the combustion chamber charge for piston position 4° CA after TDC.

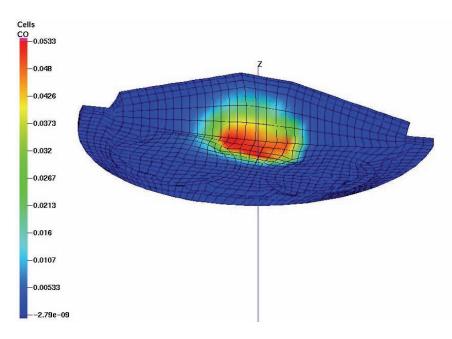


Fig. 6. Mass fraction of CO in cylinder charge at piston position 4° CA after TDC

In the above given illustration a zone of increased carbon monoxide concentration is observed in the central part of the combustion chamber. This overlaps the region of enriched mixture in connection of injection of fuel ignition dose.

Figure 7 presents distribution of mass fraction of nitric oxide in the combustion chamber for piston position 8° CA after TDC.

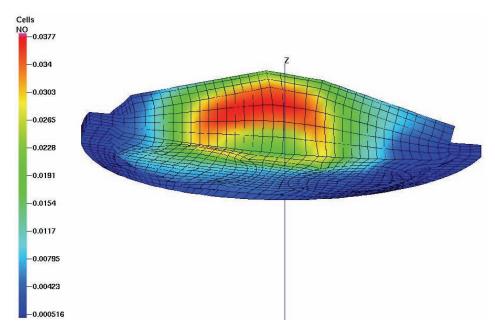


Fig. 7. Mass fraction of nitric oxide in cylinder charge for piston position 8° CA after TDC

The region of increased nitric oxide concentration lies to the central part of the combustion chamber what overlaps the zone from which the combustion process develops and where the cylinder charge reaches the highest temperature. Distribution of nitric oxide fraction in case of charge expansion at piston position 81° CA after TDC is shown in Fig. 8.

Higher mass fraction of nitric oxide is observed in ignition dose-range zone where the temperature of cylinder charge is higher.

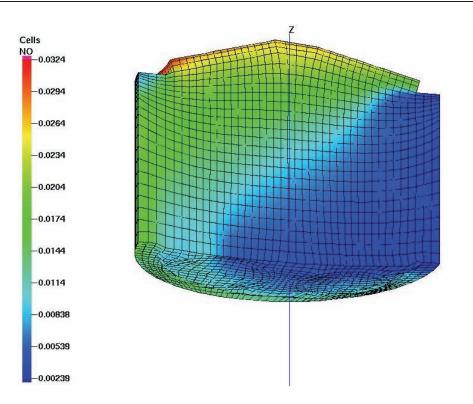


Fig. 8. Mass fraction of nitric oxide in cylinder charge at piston position 81° CA after TDC

# 4. Conclusions

The performed simulation of work cycle of the test engine indicates at possibility of mixture ignition by use of a pilot dose injected directly into the cylinder. Analysis of results of the simulation and visualisation of the combustion process showed following regularities:

- 1. Hydroxyl radicals OH initiating the combustion process are formed irregularly what is caused by charge movement in the cylinder,
- 2. In consequence of quick raise of the pressure a considerable increase in mass fraction of nitric oxide NO takes place in the cylinder to over 10 000 ppm,
- 3. The assumed fuel dosing results in absence of CO at the end of the combustion process.

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