STRATIFIED CHARGE COMBUSTION MODEL INCLUDING NO$_X$ FORMATION

Kazimierz Lejda, Paweł Woś

Rzeszów University of Technology
al. Powstańców Warszawy 8, 35-959 Rzeszów, Poland
tel.: +48 17 8651805, fax: +48 17 8543112
e-mail: klejda@prz.edu.pl, pwos@prz.edu.pl

Abstract

The paper presents a brief of mathematical model describing a two-zone, quasi-dimensional combustion in Diesel engine chamber. In order to simulate NO$_X$ emission, the simplified Zeldovitch mechanism was applied in nitric oxide formation model. An outline of the model can also be applied for engines of other types, where stratified charge is formed, e.g. in GDI spark ignition engines. In case of Diesel engines with direct fuel injection, the model includes injection sub-model that allows investigation of injection rate effect on NO$_X$ emission. This important advantage may be very useful for pre-fixing injection strategy in Common-Rail systems prior test bed fine research.

Keywords: stratified charge combustion, mathematical modeling, NO$_X$ emission, fuel injection model

1. Introduction

In combustion engine exhaust a lot of toxic compounds such as carbon monoxide CO, hydrocarbons HC, nitric oxides NO$_X$, particles PM, and many others can be found. Most of them might be easily eliminated in exhaust system by use of filters and catalytic converters. But some might be not. It goes for NO$_X$. The main cause of NO$_X$ formation is presence of oxygen O$_2$ and nitrogen N$_2$ molecules in combustion zone in the cylinder. There, during combustion, in very high temperature, a dissociation process occurs and free atoms of nitrogen and oxygen are released. These atoms are characterized by very high chemical activity and get quickly in reaction each other and with rest of N$_2$ and O$_2$ molecules, what results in NO and NO$_2$ formation. This is mainly thermal process - the higher combustion temperature the higher NO$_X$ formation rate [4].

The NO$_X$ formation during in-cylinder combustion with atmospheric air can't be avoided. However, it can be limited by two manners - to affect combustion process in such a way that excessive growth of NO$_X$ emission should not be allowed; or to eliminate just formed NO$_X$ from exhaust by a catalytic converter. The second way is used for homogenous charge, stoichiometric combustion engines rather. In diesel engines and other ones, where stratified charge, lean combustion proceeds, use of standard three-way catalytic converters does not give a good results because of high exhaust oxygen concentration. Thus, the most suitable and almost the only manner to limit NO$_X$ emission for this type of engines seems to be a proper regulation of the combustion process.

The working cycle in the piston engines is very complex, especially a combustion stage, when many phenomena combine together in the same time and area. For example, in Diesel engines simultaneously occurs injection, fuel atomization and vaporization, induction of ignition, burning and many others chemical processes. All of them take only a few milliseconds. That is why full combustion optimization needs performing a lot of time- and fund-consuming experimental tests. The injection process has a fundamental influence on combustion, and finally on performance and ecological parameters of the engine. Knowledge of these mechanisms should allow helping in

combustion control. It can be achieved not only in experimental way, but also by mathematical modeling of engine working cycle. Additionally, analytical methods allow fully arbitrary analyzing and are more time and cost efficient.

2. Description of a combustion model

All working cycle mathematical models can be sorted as follows [5]:
1) as regards dimensions, we have:
    - zero-dimensional models,
    - quasi-dimensional models,
    - multi-dimensional models;
2) as regards number of marked zones, we have:
    - one-zone models,
    - two-zone models,
    - multi-zone models.

Above segmentation defines a model complexity and fidelity in reflection of reality in the model. It is also connected with complication in mathematical tools used for simulation. The fundamental problem to select a proper type of the model is to agree to a compromise between accuracy and labor consumption needed to describe all phenomena. A priority here is the goal of analysis. As a rule, for comparative and/or quantitative research, a simplified model can be used giving good results; for qualitative investigations more precise model should be worked out instead.

Here will be presented an example of two-zone, quasi-dimensional model of combustion applied for DI Diesel engine. Split of the combustion chamber into two zones, although complicates a mathematics, yet makes much better fidelity in representation of phenomena proceeded inside the cylinder of this type of the engine. The scheme of physical and chemical processes is shown on Fig. 1.
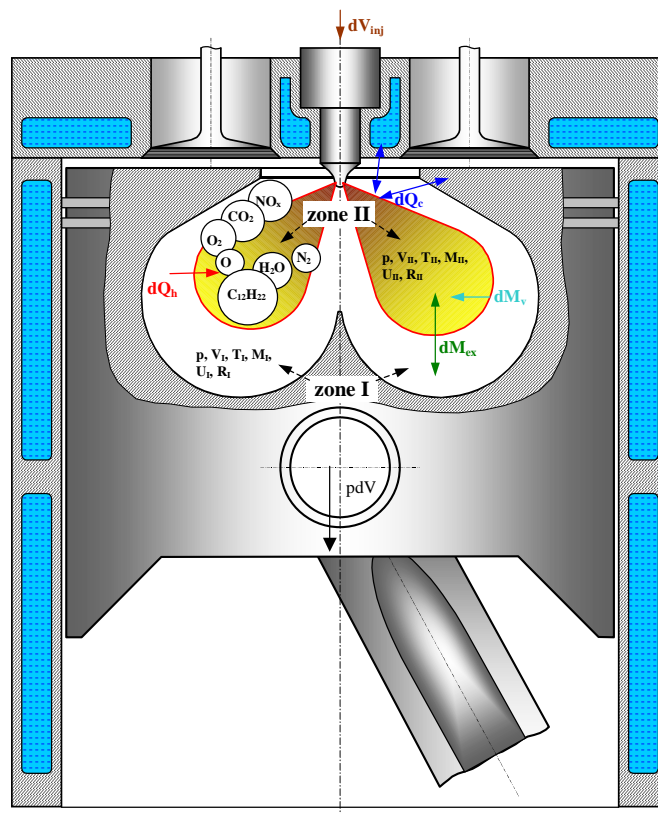

Fig. 1. The scheme of physical and chemical processes proceeded in combustion chamber in DI Diesel engine [6] (denotations are explained in the chapter below)

Inside the cylinder of volume V and pressure p, where at the end of intake stroke there is a fresh charge of a mass M_{ch}, at the moment determined by the start of injection angle a fuel dose begins to be injected. The fuel volume flow rate is $dV_{inj}/d\varphi$. Here, $d\varphi$ means increment of an independent variable of crank angle. A part of the fuel begins to evaporate with the rate equals $dM_v/d\varphi$. It forms streams of fuel-air mixture of total volume V_{II}. Through that, the combustion chamber is divided on two zones: the first one (I) of rest of fresh charge, and the second one (II) of fuel-air mixture. After short time of autoignition delay τ_o, process of evaporated fuel combustion begins with the burning rate equals $dM_h/d\varphi$. It results in a heat flux $đQ_h/d\varphi$ that is supplied into the zone II. Between both zones (I and II) mass transfer occurs ($dM_{ex}/d\varphi$), similarly between cylinder walls and both zones heat transfer of the rate $đQ_c/d\varphi$ occurs. The whole system gives an elementary mechanical work equals $pdV/d\varphi$. Except of fundamental combustion reaction, in both zones process of dissociation of some compounds runs, as well as NO_X formation. Finally, seven chemical species are considered.

On the basis of above physical model, taking indispensable assumptions into consideration, a mathematical model of engine working cycle was formulated. The essential equation for energy conversion inside the cylinder is differential equation of the first law of thermodynamics for open systems:

$$\frac{dU}{d\varphi} = \frac{đQ}{d\varphi} - p\frac{dV}{d\varphi} + \frac{dH}{d\varphi} \tag{1}$$

where:

U - internal energy of the system [J],
Q - heat delivered to/derived from the system [J],
V - system volume [m^3],
p - system pressure [Pa],
H - enthalpy delivered to/derived from the system [J],
φ - crank angle [deg].

Above equation is valid for both zones, and for both must be developed further. According to the assumptions taken in the physical model, we can write (detailed evaluation can be found in [6]):

- for heat fluxes:

$$\frac{đQ_I}{d\varphi} = -\frac{đQ_{cI}}{d\varphi} \qquad \text{and} \qquad \frac{đQ_{II}}{d\varphi} = -\frac{đQ_{cII}}{d\varphi} + \frac{đQ_h}{d\varphi} - \frac{đQ_v}{d\varphi} \tag{2}$$

- for mass transfers:

$$\frac{dM_I}{d\varphi} = \frac{dM_{ex}}{d\varphi} \qquad \text{and} \qquad \frac{dM_{II}}{d\varphi} = \frac{dM_v}{d\varphi} - \frac{dM_{ex}}{d\varphi} \tag{3}$$

- and for enthalpy fluxes:

$$\frac{dH_I}{d\varphi} = h_{ex} \cdot \frac{dM_{ex}}{d\varphi} \qquad \text{and} \qquad \frac{dH_{II}}{d\varphi} = h_v \cdot \frac{dM_v}{d\varphi} - h_{ex} \cdot \frac{dM_{ex}}{d\varphi} \tag{4}$$

where:

I, II   - subscripts referred to zone I and II in order,
Q_c - heat of cooling [J],
Q_h - heat generated by combustion [J],
Q_v - heat consumed by vaporizing fuel [J],
M_{ex} - mass transferred between both zones [kg],
M_v - mass of evaporated fuel [kg],
h_{ex} - specific enthalpy of transferred mass; it is specific enthalpy of I or II zone depending on direction of mass flow [J/kg],
h_v - specific enthalpy of fuel vapor [J/kg],

Total internal energy of any thermodynamic system can be expressed by multiplying specific internal energy *u* and system mass *M*. Thus, we can also differentiate this multiplication, what gives:

$$\frac{dU}{d\varphi} = \frac{d(M \cdot u)}{d\varphi} = u \cdot \frac{dM}{d\varphi} + M \cdot \frac{du}{d\varphi} \tag{5}$$

If we consider, that specific internal energy *u* for various compounds mixture can be calculated as $u = \sum_i (u_i \cdot g_i)$ then, assuming $\sum_i \left(u_i \cdot \frac{dg_i}{d\varphi} \right)$ is almost zero, we get:

$$\frac{du}{d\varphi} = \frac{dT}{d\varphi} \cdot \sum_i \left(g_i \cdot \frac{\partial u_i}{\partial T} \right) \tag{6}$$

where:

u_i - specific internal energy for a "*i*"component [J/kg],
g_i - mass fraction of a "*i*" component in whole system [kg/kg],
T - system temperature [K].

After substitution all above equations into the fundamental equation (1) for both zones, we get a system of two differential equations with three unknowns: $dT_I/d\varphi$, $dT_{II}/d\varphi$, and $dM_{ex}/d\varphi$:

$$\begin{cases} \left[\sum_i (u_{Ii} g_{Ii}) - h_{ex} \right] \frac{dM_{ex}}{d\varphi} + M_I \sum_i \left(g_{Ii} \frac{\partial u_{Ii}}{\partial T} \right) \frac{dT_I}{d\varphi} = \frac{dQ_I}{d\varphi} - p \frac{dV_I}{d\varphi} \\[4mm] \left[h_{ex} - \sum_i (u_{IIi} g_{IIi}) \right] \frac{dM_{ex}}{d\varphi} + M_{II} \sum_i \left(g_{IIi} \frac{\partial u_{IIi}}{\partial T} \right) \frac{dT_{II}}{d\varphi} = \frac{dQ_{II}}{d\varphi} - p \frac{dV_{II}}{d\varphi} - \left[\sum_i (u_{IIi} g_{IIi}) - h_v \right] \frac{dM_v}{d\varphi} \end{cases} \tag{7}$$

The other differentiates, such as $dQ_I/d\varphi$, $dQ_{II}/d\varphi$, $dV_I/d\varphi$, $dV_{II}/d\varphi$, $dM_v/d\varphi$, can be calculated using separated sub-models. To resolve above system algebraically, $dM_{ex}/d\varphi$ must be eliminated and expressed by other known components. To do that, we use an overall assumption that pressure *p* in both zones is equal:

$$p_I = p_{II} \tag{8}$$

According to ideal gas law equation of Clapeyron it also means that:

$$\frac{M_I \cdot R_I \cdot T_I}{V_I} = \frac{M_{II} \cdot R_{II} \cdot T_{II}}{V_{II}} \tag{9}$$

where the symbols refer to both zones, such as subscript indicates, and there are:

M - mass of the zone [kg],
R - universal gas constant for whole zone [J/(kg·K)],
T - average temperature of the zone [K],
V - zone volume [m^3].

Going ahead, at any time a mass of the first zone is a sum of initial mass of fresh charge M_{ch} and transferred mass M_{ex}, and for the second one it is a mass of evaporated fuel M_v from which transferred mass M_{ex} is subtracted. Then transferred mass can be evaluated as follows:

$$M_{ex} = \frac{M_v \cdot R_{II} \cdot T_{II} \cdot V_I - M_{ch} \cdot R_I \cdot T_I \cdot V_{II}}{R_I \cdot T_I \cdot V_{II} + R_{II} \cdot T_{II} \cdot V_I} \tag{10}$$

To differentiate it relatively to crank angle variable φ, we receive a formula for component $dM_{ex}/d\varphi$ as a function expressed by the other differentiates:

$$\frac{dM_{ex}}{d\varphi} = f\left(\frac{dT_I}{d\varphi}, \frac{dT_{II}}{d\varphi}, \frac{dV_I}{d\varphi}, \frac{dV_{II}}{d\varphi}, \frac{dM_v}{d\varphi} \right) \tag{11}$$

Now, replacing the component $dM_{ex}/d\varphi$ in the system of equations (7) with the above function we receive a new system of two differential equations with two unknowns $dT_I/d\varphi$, $dT_{II}/d\varphi$ only, i.e.:

$$\begin{cases} A \cdot \dfrac{dT_I}{d\varphi} + B \cdot \dfrac{dT_{II}}{d\varphi} = C \\ D \cdot \dfrac{dT_I}{d\varphi} + E \cdot \dfrac{dT_{II}}{d\varphi} = F \end{cases} \tag{12}$$

where A, B, C, D, E, F contains expressions of known variables, which can be evaluated by use of separated sub-models and/or formulas. In this shape of the system, the unknowns $dT_I/d\varphi$, $dT_{II}/d\varphi$ can not be calculated by any of numerical methods. These methods need explicit from of equations. To get it, the system (12) has to be transformed (solved algebraically) relatively to $dT_I/d\varphi$, $dT_{II}/d\varphi$. For instance, applying the method of Cramer determinants we have:

$$\begin{cases} \dfrac{dT_I}{d\varphi} = \dfrac{B \cdot F - E \cdot C}{B \cdot D - E \cdot A} \\ \dfrac{dT_{II}}{d\varphi} = \dfrac{C \cdot D - A \cdot F}{B \cdot D - E \cdot A} \end{cases} \tag{13}$$

Above computer simulation friendly form of equations has been implemented to perform all calculations.

In the model of NO_X formation, the two of reversible Zeldovitch's reactions have been used [1, 2]:

$$O + N_2 \quad \leftrightarrow \quad NO + N \tag{14}$$
$$N + O_2 \quad \leftrightarrow \quad NO + O \tag{15}$$

On the base of chemical kinetic theory, the formula to calculate the NO formation rate according to the above reaction scheme is following:

$$\frac{1}{V} \cdot \frac{dn_{NO}}{dt} = 2k_1[O][N_2] \tag{16}$$

where:

V - volume of reaction zone [m^3],
n_{NO} - mole number of NO [mole],
t - time [s],
k_1 - kinetic constant of the first Zeldovitch reaction in forward direction [m^3/(mole·s)],
[O], [N_2] - molar concentration of O-atoms and N_2-molecules inside the reaction zone [mole/m^3].

It follows that the formation rate is controlled by the first reaction of Zeldovitch. Atoms of oxygen come mainly from dissociation $O_2 \leftrightarrow 2\,O$, and its concentration can be calculated as follows:

$$[O] = \left(K^c{}_O \cdot [O_2] \right)^{\frac{1}{2}} \tag{17}$$

where:

$K^c{}_O$ - equilibrium constant of oxygen dissociation reaction referred to the concentration [mole/m^3],
[O], [O_2] - molar concentration of O-atoms and O_2-molecules inside the reaction zone [mole/m^3].

Finally, the NO formation rate formula (16) takes following shape (all denotations are as same as above):

$$\frac{1}{V} \cdot \frac{dn_{NO}}{dt} = 2k_1 \cdot K^c{}_O{}^{\frac{1}{2}} \cdot [O_2]^{\frac{1}{2}} \cdot [N_2] \tag{18}$$

The same formula can express a mass flux of NO in kilograms, such as to be used directly in model equations. It should be changed as follows:

$$\frac{dM_{NO}}{d\varphi} = \frac{\mu_{NO} \cdot V}{6000 \cdot n} \cdot \left[2k_1 \cdot K^c{}_O{}^{\frac{1}{2}} \cdot [O_2]^{\frac{1}{2}} \cdot [N_2] \right] \tag{19}$$

where:

μ_{NO} - molar mass of nitric oxide [g/mole]; $\mu_{NO} = 30,0061$,
n - engine speed [rev/min],
      - remaining denotations are as same as above.

The constants $K^c{}_O$ and k_1 can be gathered from the bibliography sources [1, 5], and were slightly modified to achieve validated results. The initial values of them can be equal to:

$$k_1 = 7{,}6 \cdot 10^7 \cdot exp\left(\frac{-38000}{T}\right) \left[\frac{m^3}{mole \cdot s}\right] \tag{20}$$

$$K^c_O = \frac{10^{5+0{,}310805 \cdot ln(T) - \frac{12954}{T} + 1{,}07083 - 0{,}738336 \cdot 10^{-4} \cdot T + 0{,}344645 \cdot 10^{-8} \cdot T^2}}{\overline{R}T} \left[\frac{mole}{m^3}\right] \tag{21}$$

3. Model estimation and calculation results

Described in brief, the model has been validated using a test stand. The stand was supported by the single-cylinder, direct injection diesel engine SB 3.1. The full scheme of the bench is shown on Fig. 2.
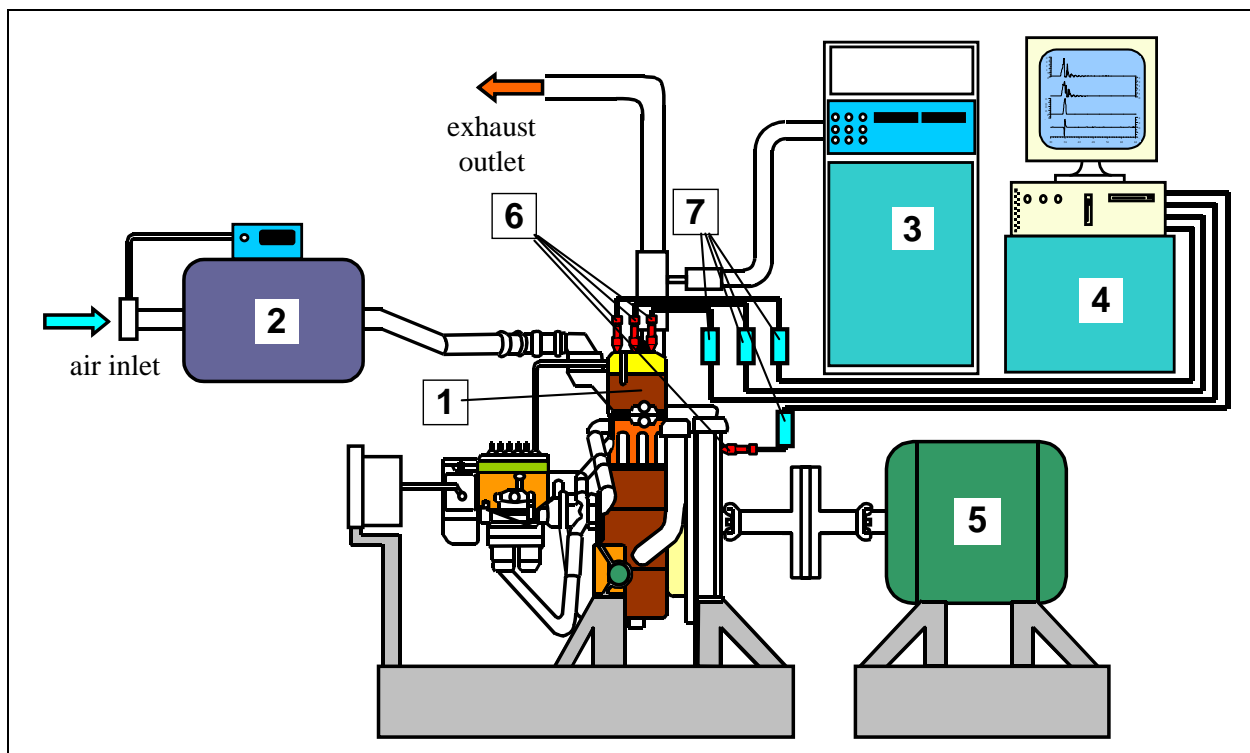

Fig. 2. The scheme of the test bench [3]: 1 - test engine SB 3.1, 2 - air consumption meter, 3 - Pierburg NOx analyzer, 4 - control computer with fast data acquisition card, 5 - eddy-current dynamometer, 6 - AVL pressure, lift, and crank angle sensors, 7 - amplifiers

The main acquired parameters were: injector needle lift, fuel pressure before the injector, pressure inside the combustion chamber, exhaust concentration of NO_X, and fuel and air consumption. The injector needle lift and fuel pressure data were used to calculate fuel injection rate, and NO_X concentration and exhaust flux data were used to calculate NO_X emission.

Some of parameters in the model have had to be tuned up to achieve satisfactory conformity between calculated results and experiments. It is common feature of all semi-empirical models and cannot be avoided in the process of parameter estimation. The sample results (Fig. 3) show that the convergence in the field of NO_X emission was not worse than 10%. It can be considered as a good result, seeing that the model contains many simplifications and assumptions.
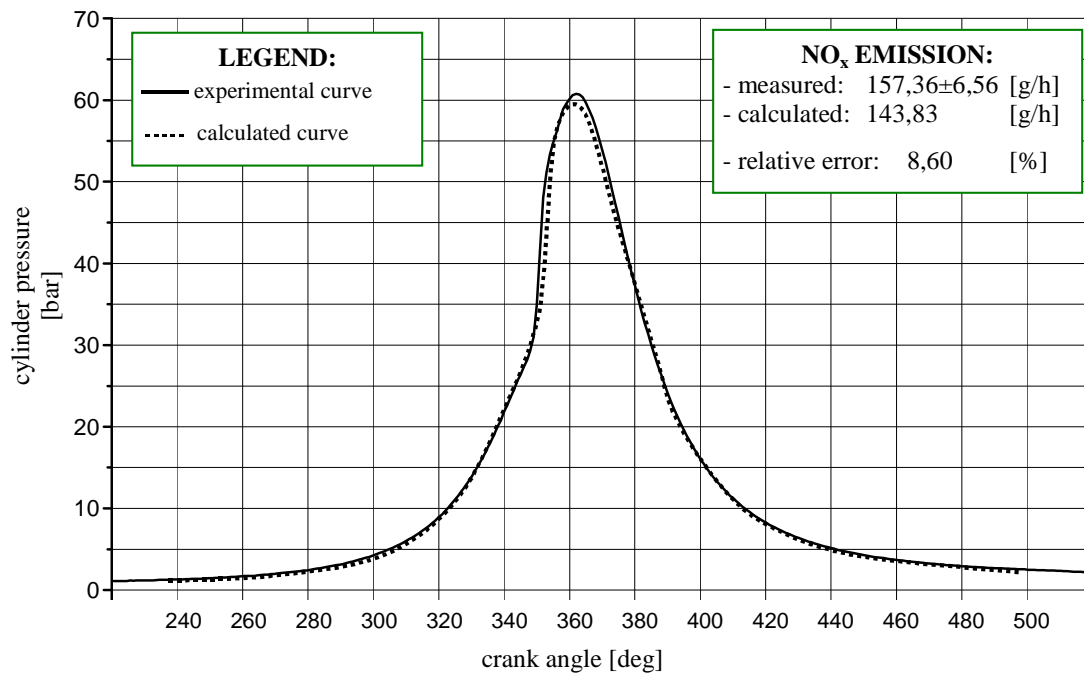
Fig. 3. Experimental and simulated results comparison [6] (engine speed n = 1000 rev/min, half load)

4. Conclusion

The mathematical model of combustion presented in the paper includes a lot of phenomena. Here, from among of rich set, only the formulas for thermodynamic energy conversion and NO_X formation were selected for presentation. Many of physical and chemical effects occurred in reality have been omitted in the model or included in reduced form because of impossibility in exact mathematical representation. Surely, it influences model accuracy, but is also partially compensated in parametric estimation process. This way of model validation has the disadvantage that must be anew performed for each engine taken into simulation. Nevertheless, the model is a valuable research tool, which can be used for extensive studies of combustion in stratified charge engines.

References

[1] Heywood, J. B., *Internal Combustion Engines Fundamentals,* McGraw Hill Co., New York 1988.
[2] Kafar, I., Piaseczny, L., Merkisz, J., *Mathematical Model of Toxic Compound Emissions in Exhaust Gases Produced by Marine Engines,* Journal of KONES, vol. 5, No 1, Warsaw - Gdańsk 1998.
[3] Lejda, K., Woś, P., *Effect of fuel injection rate on NO_X emission in Diesel engine*. Machine Engineering, vol. 8, book 4, Publishing Agency of Wroclaw Board of FSNT NOT, Wrocław 2003, (in Polish).
[4] Merkisz J., *Ecological Problems of Combustion Engines*. Publishing by Poznań University of Technology, Poznań 1999, (in Polish).
[5] Rychter, T, Teodorczyk, A., *Mathematical Modeling of Piston Engine Working Cycle,* PWN, Warsaw 1990, (in Polish).
[6] Woś, P., *An Analysis of Fuel Injection Rate Effect on NO_X Emission from Direct Injection Diesel Engine,* Doctor Thesis, Rzeszów University of Technology 2003, (in Polish).