We are IntechOpen, the world's leading publisher of Open Access books Built by scientists, for scientists

4,800
Open access books available

122,000
International authors and editors

135M
Downloads

Our authors are among the

154
Countries delivered to

TOP 1%
most cited scientists

12.2%
Contributors from top 500 universities

CLARIVATE ANALYTICS BOOK CITATION INDEX INDEXED

WEB OF SCIENCE™

Selection of our books indexed in the Book Citation Index in Web of Science™ Core Collection (BKCI)

Interested in publishing with us?
Contact book.department@intechopen.com

Numbers displayed above are based on latest data collected.
For more information visit www.intechopen.com

4

Simulation of Combustion Process in Direct Injection Diesel Engine Based on Fuel Injection Characteristics

Kazimierz Lejda and Paweł Woś
Rzeszów University of Technology
Poland

1. Introduction

Combustion engines are still the major propulsion devices for many mechanical equipment including mostly all automotive vehicles. Unfortunately, they negatively affects natural environment due to exhaust gas emission consisting of harmful compounds, like the carbon monoxide CO, unburned hydrocarbons HC, nitric oxides NO and NO_2 (altogether marked as NO_X), solid particles PM, and finally the carbon dioxide CO_2, that is to blame for the global warming phenomenon. All of them may cause human health deterioration or unwanted changes in the atmosphere in a large scale. As the examples, formation of the photochemical smog where hydrocarbons and oxides of nitrogen play the main role, or destruction of the ozone protective layer with participation of nitric oxide can be pointed here. There are also many other compounds in the exhaust gases which, besides their eco-toxicity, show also a serious carcinogenic action against people and animals, e.g. some hydrocarbons and particulate matter fractions.

The prevention-natured, legislative limitations of vehicle exhaust emission stemmed from these threats, together with the current and prospective growth of road transportation intensity, calls for continuous effort to develop vehicle powertrains that must be done both in design and technology domains. Hence the combustion engine improvement works have been spreading out within the space of last decades, and now they consider more and more factors. They pursue a simultaneous decreasing of harmful exhaust emission (CO, HC, NO_X, PM) and fuel consumption. Particularly, the thing is to cut down on CO_2 emission by increasing engine total efficiency. Fulfilling all above tasks encounters many problems. They contradict each other, what originates from complex physical and chemical interactions during the working cycle of piston engines, especially at combustion stage, where many phenomena combine together in the same time and area. For example, in direct injection engines simultaneously occurs: injection, fuel atomization and vaporization, induction of ignition or autoignition, fuel burning and many other chemical processes. All it takes only a few milliseconds. That is why improving exhaust emission parameters usually claims resignation from good fuel efficiency, and vice versa, fuel consumption decreasing escalates harmful emission. Hence, it is necessary to perform a lot experimental research in order to find an optimal solution. Unfortunately, they are generally complicated and expensive, but they could be successfully supported by numerical simulation. By the way, computational

methods allow boundary-free analyzing and may narrow the range of further experiments. They are also much more time and cost-efficient than test bed investigations.

Fuel injection in combustion engines belongs to the most important working processes. Particularly, in direct injection (DI) engines, both gasoline and diesel one, it truly triggers and controls combustion, influencing all output engine performances together with exhaust emissions. Thus, improving of combustion engines should always consider fuel injection optimization, before other kinds of engine processes are being tested. Techniques harnessing mathematical simulations are the good ways to do this in the first stage. Such approach will be shown further.

2. The background of fuel injection process and its impact on combustion

Obtaining the desired operational engine parameters like break mean effective pressure (BMEP), overall engine efficiency, or environmental indexes (exhaust emissions, noise), essentially depends on the combustion rate, and previously on formation of flammable mixture. It particularly comes true in case of a direct injection engine. As far as a quality of combustible mixture is concerned, both the appropriate fuel atomization and fuel mixing with the air charge is important here, just as the precise metering of fuel amount injected in every cycle, and providing equal amounts of fuel for each cylinder of the engine. In direct injection engines, a fuel injection system has the main responsibility for creating proper fuel-air mixture, which can be characterized by an appropriate macro- and microstructure. Air swirl has a minor importance here, or even can make the whole process worsened due to cylinder wall wetting possibility.

On the whole, the mere combustion process is sensitive to many factors which may be classified into four groups (Wajand, 1988):

- physical and chemical properties of fuel, e.g. fractional and chemical composition, cetane/octane number, temperature of fuel (auto)ignition, etc;
- structural properties of the engine, e.g. combustion chamber shape, main engine dimensions, compression ratio, materials used, etc;
- operation and regulation conditions of the engine: rotational speed of the crankshaft, engine load, ignition (or start of injection) timing, etc;
- fuel injection system layout that generates fuel delivery process with the specific fuel spray parameters; it influences directly combustion rate, as is discussed above.

These considerations indicate that the fuel injection parameters are important factors affecting combustion process and consequently the engine parameters, what has been also verified by experimental studies (Kuszewski & Szlachta, 2002; Zabłocki, 1976).

A process of fuel injection into the engine cylinder might be described by parameters related to injection rate and spray characteristics. The set of injection rate parameters consists of:

- start of injection (SOI) timing referred to crankshaft position angle [deg],
- injection duration referred to crankshaft rotation angle [deg],
- mean flow rate of the fuel in a whole injection duration [mm^3/deg],
- actual fuel injection rate (instantaneous fuel flow velocity) [mm^3/deg],
- maximum fuel flow velocity [mm^3/deg].

Presently, the pressure-accumulative fuel systems with electronically controlled injectors are widely used, e.g. Diesel common rail (CR) one. In such systems, the injection rate essentially depends on two parameters: the shape of electrical signals in the injector and the hydraulic-mechanical characteristic of the injector. The change of pressure in the fuel storage is so small and affects fuel injection rate so little that it can be neglected in simulation works on engine operation.

The fuel spray characteristics may be described by the following parameters:

- spray tip velocity and penetration,
- spray tip angle,
- fuel atomization quality expressed by mean diameter of droplets and its dispersion,
- distribution of fuel mass along and across the spray,
- equivalent mean droplets size: linear, areal, volumetric, areal-volumetric (Sauter).

Preparation of flammable mixture in a direct injection engine becomes involved not only with strategy of fuel delivery, but also with areal distribution of fuel in the cylinder space. It should be noticed that a lot of factors influencing the fuel injection rate also plays an important role in fuel atomization quality, resulting in fuel mixing with air inside the cylinder.

3. Demonstration of combustion model

All mathematical models of combustion engine working cycle can be sorted as follows (Rychter & Teodorczyk, 1990):

1. considering dimensions, we have:
- zero-dimensional models,
- quasi-dimensional models,
- multi-dimensional models;
2. considering a number of recognized zones, we have:
- one-zone models,
- two-zone models,
- multi-zone models.

Above segmentation defines a model complexity and fidelity in representation of real processes in the model. It is also connected with complication in mathematical tools used for simulation. There are a lot of examples which combines the models according to the above segmentation (Khan et. al., 1973; Patterson, 1994, 1997; Rychter & Teodorczyk, 1990). The fundamental problem in choosing a proper type of the model is to find a compromise between accuracy and intellectual labor involved to describe all physical phenomena. A priority here is the goal of analysis. As a rule, for comparative and/or quantitative research, a simplified model can be used with receiving good results; for qualitative investigations more precise model should be worked out instead.

In a preliminary analysis toward model formulating, a number of physical and chemical processes that occur during the injection, combustion and exhaust pollutant formation were taken into consideration. The latest theoretical and experimental results were regarded. A great effort was made to include to the analysis all phenomena that have a major impact on the various processes modeled, so as their actual nature would be reproduced. Thanks to

this, the model enables to simulate the effect of many structural and operational factors on the engine performance, including detailed emissions.

As a result, a two-zone quasi-dimensional model has been developed. Comparing to single-zone models, the own one is characterized by a much more accurate description of the phenomena in a combustion chamber. This attribute greatly emphasizes the scientific and utilitarian aspect of such a solution. In addition, the model permits to be extended easily of additional, computational blocks. In this respect, the proposed method of analysis exemplifies an important cognitive value and is rarely found in the literature.

Below, an application of worked out, two-zone, quasi-dimensional model of combustion for direct injection diesel engine will be presented. Splitting the combustion chamber into two zones for models of such type of the engines makes a fidelity in representation of phenomena proceeded inside the cylinder much precise, although it complicates mathematics.

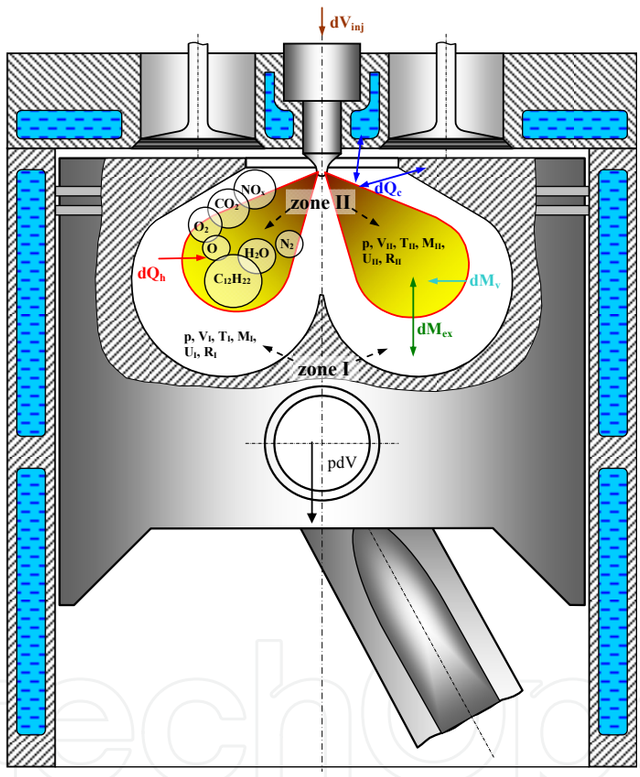


Fig. 1. The scheme of physical and chemical processes proceeded in a combustion chamber of direct injection (DI) diesel engine (Woś, 2008)[1]

As is shown in the Fig. 1, inside the cylinder of volume V and pressure p, at the end of intake stroke there is a fresh air charge of a mass M_{ch}, and at the moment determined by the start of injection angle, an initial fuel quantity begins to be injected. The fuel volume flow rate is $dV_{inj}/d\varphi$. Here, $d\varphi$ means the increment of an independent variable that is the crankshaft angle. A part of the fuel begins to evaporate with the rate equals to $dM_v/d\varphi$. It forms the spray cones of total volume V_{II}, consisted of fuel-air mixture. Through that, the

[1] The denotations are explained in the chapter body.

combustion chamber is divided onto two zones: the first one (I) - consisting of the rest of fresh charge, and the second one (II) - drawn by fuel-air mixture boundaries. After short time of autoignition delay τ_o, the process of evaporated fuel combustion gets set on and runs with the burning rate equals to $dM_h/d\varphi$. It generates a heat flux $đQ_h/d\varphi$ that is supplied into the zone II. Between both zones (I and II), a mass transfer process occurs ($dM_{ex}/d\varphi$), and between cylinder walls and both zones a heat transfer process occurs also with the rate $đQ_c/d\varphi$. The whole system gives an elementary mechanical work equals to $pdV/d\varphi$. Except of fundamental combustion reaction, the other free selected ones can be implemented (dissociations, pollutant formation) in order to check various engine output parameters.

3.1 The model core based on thermodynamic theory

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

$$\frac{\mathrm{d}U}{\mathrm{d}\varphi} = \frac{\eth Q}{\mathrm{d}\varphi} - p\frac{\mathrm{d}V}{\mathrm{d}\varphi} + \frac{\mathrm{d}H}{\mathrm{d}\varphi} \tag{1}$$

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 of the elaborated model, but it must be developed further in order to calculate temperature change in both zones. According to the assumptions taken in the physical model, we can write as follows (detailed evaluation can be found in (Woś, 2008)):

for heat fluxes:

$$\begin{aligned} \frac{\eth Q_I}{\mathrm{d}\varphi} &= -\frac{\eth Q_{c\,I}}{\mathrm{d}\varphi} \\ \frac{\eth Q_{II}}{\mathrm{d}\varphi} &= -\frac{\eth Q_{c\,II}}{\mathrm{d}\varphi} + \frac{\eth Q_h}{\mathrm{d}\varphi} - \frac{\eth Q_v}{\mathrm{d}\varphi} \end{aligned} \tag{2}$$

for mass transfers:

$$\begin{aligned} \frac{dM_I}{d\varphi} &= \frac{dM_{ex}}{d\varphi} \\ \frac{dM_{II}}{d\varphi} &= \frac{dM_v}{d\varphi} - \frac{dM_{ex}}{d\varphi} \end{aligned} \tag{3}$$

and for enthalpy fluxes:

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

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: $u = \sum_i (u_i \cdot g_i)$; then, assuming $\sum_i \left(u_i \cdot \frac{dg_i}{d\varphi} \right)$ as near to null, we will 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 an "i" component [J/kg],

g_i-mass fraction of an "i" component in a whole system [kg/kg],

T-temperature of the system [K].

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

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

The other differentiates, such as $đQ_{\mathrm{I}}/\mathrm{d}\varphi$, $đQ_{\mathrm{II}}/\mathrm{d}\varphi$, $\mathrm{d}V_{\mathrm{I}}/\mathrm{d}\varphi$, $\mathrm{d}V_{\mathrm{II}}/\mathrm{d}\varphi$, $\mathrm{d}M_{\mathrm{v}}/\mathrm{d}\varphi$, can be calculated with use of independent submodels. To resolve above system algebraically, $\mathrm{d}M_{\mathrm{ex}}/\mathrm{d}\varphi$ must be eliminated and expressed by other known components. To do that, we can use an overall assumption that the pressure p in both zones is always equal in value:

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

According to the 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 they mean as follows:

M–mass of the zone [kg],

R–universal gas constant for a whole zone [J/(kg·K)],

T–average temperature of the zone [K],

V–zone volume [m^3].

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

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

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

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

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

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

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

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

Above computer simulation friendly form of equations can be already implemented into the numerical calculation package and allow program running. Obviously, this core model has to be added with necessary sub-models describing other phenomena like heat transfer, fuel injection, fuel atomization and evaporation, ignition delay, combustion rate, combustion products formation, etc. The chosen ones will be shown further.

3.2 Fuel injection model

Modeling of the fuel injection in the combustion chamber space is one of the most difficult issues in all simulation works regarding the processes in reciprocating combustion engines. This is caused mainly by limited expertise knowledge in this field. Thus, in simulation works covering the combustion chamber space, a representation level of fuel injection submodel, as well fuel evaporation and combustion one is assumed with consideration of total accuracy of the whole model. More complex, spatial mathematical description should be used only in the cases where the injection process is the main essence of modeling.

In the current study, a number of simplifying assumptions in description of the fuel injection process have been made. Nevertheless, they were tailored to the level of accuracy in whole zero-dimensional model layout. According to the preliminary analysis, it has been assumed that the distribution of fuel density in the sprays generated is the same in all directions; next, the shape of sprays is characterized by a constant tip angle, and spray microstructure is described by the mean droplet diameter according to Sauter definition (SMD – Sauter Mean Diameter) and it is uniform throughout the entire space of fuel jet.

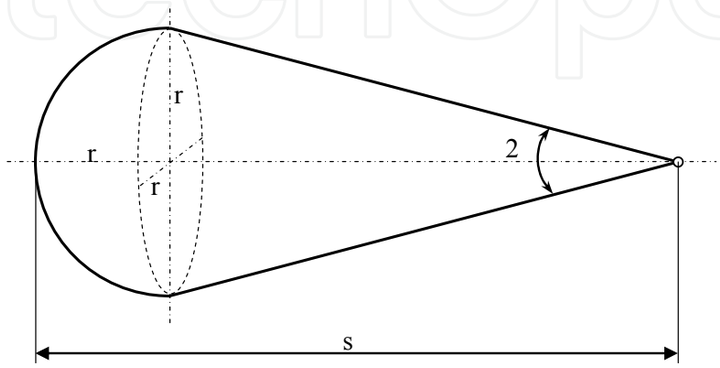


Fig. 2. A model for single fuel spray geometry (Woś, 2008)

According to the physical model layout that is shown in Fig. 1, the geometry of fuel injection sprays defines the volume of the zone of fuel-air mixture signed as zone II. A following simplified single spray cone geometry model has been adapted (Fig. 2).

Spray tip penetration *s* and tip angle 2α are the principal parameters. They allow calculating the volume of zone II (V_{II}) by multiplying the volume of elementary spray and number of sprays generated by the injector, i.e. the number of holes in the sprayer *i*:

$$\begin{aligned} V_{II}(\varphi) &= i \cdot \left[\frac{1}{3}\pi \cdot \left(\frac{s(\varphi)}{ctg\,\alpha + 1} \right)^2 \cdot s(\varphi) \cdot \left(1 - \frac{1}{ctg\,\alpha + 1} \right) + \frac{2}{3}\pi \cdot \left(\frac{s(\varphi)}{ctg\,\alpha + 1} \right)^3 \right] = \\ &= i \cdot \frac{1}{3}\pi \cdot s(\varphi)^3 \cdot \left[\frac{1}{(ctg\,\alpha + 1)^2} + \frac{1}{(ctg\,\alpha + 1)^3} \right] \end{aligned} \tag{14}$$

Equation (14) expresses an instantaneous volume of the zone II that varies within the injection duration. According to the assumptions made, the change of zone II volume (V_{II}) just depends on a spray tip penetration increasing d*s*/dφ:

$$\begin{aligned} \frac{dV_{II}}{d\varphi} &= i \cdot \pi \cdot s(\varphi)^2 \cdot \left[\frac{1}{(ctg\,\alpha + 1)^2} + \frac{1}{(ctg\,\alpha + 1)^3} \right] \cdot \frac{ds}{d\varphi} = \\ &= i \cdot \pi \cdot s(\varphi)^2 \cdot \left[\frac{1}{(ctg\,\alpha + 1)^2} + \frac{1}{(ctg\,\alpha + 1)^3} \right] \cdot v_s(\varphi) \end{aligned} \tag{15}$$

where the symbols used in above equations, both (14) and (15), mean:

$V_{II}(\varphi)$–total volume of combustion zone II at specified crankshaft angle position [m^3],

$dV_{II}/d\varphi$–change of total volume of zone II [m^3/deg],

i–number of holes in the sprayer [–],

s(φ)–spray tip penetration at specified crankshaft angle position [m],

$v_s(\varphi)$–spray tip velocity at specified crankshaft angle position [m/deg],

α–a half of spray tip angle [rad],

φ–independent variable: crankshaft angle position [deg].

Empirical formulas have been used for further analysis. They are based on criterion numbers that are widely used in fluid mechanics. And so, the relationship of spray tip penetration *s* and velocity v_s is given by the following formulae (Orzechowski & Prywer, 1991):

$$s(\varphi) = \sqrt{\frac{d_r \cdot w_0}{\sqrt{2} \cdot a_u} \cdot \frac{1}{6 \cdot n} \cdot \left| \varphi - \varphi_{inj} \right|} \tag{16}$$

$$v_s(\varphi) = \frac{ds}{d\varphi} = \frac{d_r \cdot w_0}{2 \cdot \sqrt{2} \cdot a_u \cdot s(\varphi)} \tag{17}$$

where:

$s(\varphi)$, $v_s(\varphi)$–spray tip penetration [m] and velocity [m/s] at crankshaft angle position φ,

d_r–spraying hole diameter [m],

n–crankshaft rotational speed [1/min],

φ–independent variable: the current crankshaft angle position [deg],

φ_{inj}–crankshaft angle position at start of injection [deg],

w_0–an initial velocity of fuel spray tip left the injector [m/s],

$$w_0 = \mu \cdot \sqrt{\frac{2 \cdot \Delta p}{\rho_f}} \tag{18}$$

μ–flow factor of the injector holes [–]; μ ≈ 0.7 according to (Orzechowski & Prywer, 1991),

Δp–pressure drop inside the sprayer [Pa],

ρ_f–fuel density [kg/m^3],

a_u–factor of free-stream turbulence in the spray tip layer [–],

$$a_u = C_1 \cdot We^k \cdot Lp^l \cdot M^m \tag{19}$$

We–dimensionless Weber criteria number [–],

$$We = \frac{\rho_f \cdot w^2 \cdot d_r}{\sigma_f} \tag{20}$$

Lp–dimensionless Laplace criteria number [–],

$$Lp = \frac{\rho_f \cdot \sigma_f \cdot d_r}{\eta_f^2} \tag{21}$$

M–air to fuel density ratio [–],

$$M = \frac{\rho_g}{\rho_f} \tag{22}$$

w–relative velocity of fuel droplets inside the spray jet [m/s]; $w = w_0$,

d_r–diameter of sprayer holes [m],

σ_f–fuel surface tension [N/m],

ρ_f–fuel density [kg/m^3],

ρ_g–cylinder charge density (air density) [kg/m^3],

η_f–fuel absolute viscosity [kg/(m·s)],

C_1, k, l, m–experimental constants (see Table 1).

For high backpressure (M = 0.0095 - 0.028)	For low backpressure (M = 0.0014 - 0.0095)
C_1= 2.72 k= −0.21 l= 0.16 m= 1	C_1= 0.202 k= −0.21 l= 0.16 m= 0.45

Table 1. The values of experimental constants *C_1, k, l, m* used for calculation of spray tip penetration (Orzechowski & Prywer, 1991)

The spray tip angle, similarly to the spray tip penetration, is the function of parallel known parameters, i.e. densities of fuel and cylinder charge (ρ_f, ρ_g), fuel absolute viscosity and surface tension (η_f, σ_f), an initial velocity of fuel spray tip left the injector (w_0), diameter of sprayer holes (d_r) and time (t). Excepting an initial phase o the injection, the spray tip angle does not change, so the effect of time axis can be neglected. Further analysis is based on the following formula:

$$\operatorname{tg} \alpha = C \cdot We^k \cdot Lp^l \cdot M^m \tag{23}$$

hence:

$$\alpha = \operatorname{arctg} (C \cdot We^k \cdot Lp^l \cdot M^m) \tag{24}$$

where:

α–a half of spray tip angle [rad],

We, Lp, M–same numbers as for equations (20)-(22),

C, k, l, m–experimental constants (see Table 2).

For high backpressure (M = 0.0095 – 0.028)	For low backpressure (M = 0.0014 – 0.0095)
C= 0.0089 k= 0.32 l= 0.07 m= 0.5	C= 0.0028 k= 0.32 l= 0.07 m= 0.26

Table 2. The values of experimental constants *C, k, l, m* used for calculation of spray tip angle (Orzechowski & Prywer, 1991)

The last but not least of the analyzed parameters that is essential for this methodology is microstructure parameter of the spray jet, i.e. mean diameter of droplets. It means an equivalent average value respecting the whole spectrum of diameters of actual droplets generated by the injector. There are a few definitions of equivalent droplet size. Each of them can be described according to the general formula:

$$d_{p,q} = \sqrt[p-q]{\frac{\sum n_i \cdot d_i^p}{\sum n_i \cdot d_i^q}} \tag{25}$$

where:

$d_{p,q}$–theoretical equivalent mean diameter of droplets in a spray jet [mm],

p, q–the exponents that correspond with adopted definition of droplet mean diameter [–]; the values of p and q and formula shape for various definitions is given in Table 3,

d_i–an actual diameter of droplet in spray jet [mm],

n_i–the number of droplets of the actual diameter d_i [–].

Equivalent mean diameter of droplets	p	q	Calculation formula
Arithmetic d_{10}	1	0	$d_{1,0} = \frac{\sum n_i \cdot d_i}{\sum n_i}$
Areal d_{20}	2	0	$d_{2,0} = \sqrt{\frac{\sum n_i \cdot d_i^2}{\sum n_i}}$
Areal comparative d_{21}	2	1	$d_{2,1} = \frac{\sum n_i \cdot d_i^2}{\sum n_i \cdot d_i}$
Volumetric d_{30}	3	0	$d_{3,0} = \sqrt[3]{\frac{\sum n_i \cdot d_i^3}{\sum n_i}}$
Volumetric comparative (Probert) d_3	3	1	$d_{3,1} = \sqrt{\frac{\sum n_i \cdot d_i^3}{\sum n_i \cdot d_i}}$
Volumetric-areal (Sauter) (also SMD - Sauter mean diameter) d_{32}	3	2	$d_{3,2} = \frac{\sum n_i \cdot d_i^3}{\sum n_i \cdot d_i^2}$

Table 3. The list of chosen definition formulas for calculation of mean diameter of droplets in a spray jet (Orzechowski & Prywer, 1991)

For combustion engine research area, the most usefulness definition is this one, given by Sauter formula $d_{3,2}$ (Table 3). It allows the most accurate rendering of the phenomena, where evaporation, heat and mass transfer, and combustion proceeds and is strictly crucial. Since the equation of SMD definition can be used only for research of mere injection process, comparative studies give different empirical formulas for calculations with using other parameters. For example, Hiroyasu and Katoda (Hiroyasu & Katoda, 1976) elaborated the experimental formula which is convenient to use in engine fuel injection and combustion studies. The equation, which has been consequently used by other researchers (Benson et. al., 1979; Heywood, 1988) is following:

$$d_{3,2} = A \cdot \Delta p^{-0.135} \ \rho_g{}^{0.121} \ q_{Vf}{}^{0.131} \tag{26}$$

where:

$d_{3,2}$–Sauter mean diameter [μm],

A–a constant for specific sprayer type [–]; for hole sprayer: A = 23.9,

Δp–fuel injection overpressure [MPa],

ρ_g–density of cylinder charge [kg/m^3],

q_{Vf}–amount of a single fuel injection volume [mm^3].

The presented methodology for calculation of fuel spray jet parameters is based on extensive experimental studies. Thus it is expected to provide a good consistence of calculated results with experiments.

3.3 Fuel evaporation model

Fuel evaporation process is a predecessor of combustion, which begins to run just after the start of injection. The evaporation rate is the function of numerous factors, both spray surroundings and the mere fuel parameters. Nevertheless, the temperature inside the combustion chamber is the most important here. For a single fuel droplet, a relationship between size decreasing and evaporation intensity is known (Kowalewicz, 2000):

$$d_0^2 - d^2 = K \cdot t \tag{27}$$

where:

K–evaporation intensity factor that depends on temperature of surrounding where the fuel is injected [mm^2/s],

t–evaporation time [s],

d_0–initial diameter of droplet [mm],

d–diameter of droplet after the time *t* [mm].

An evaporation intensity factor *K* is the function of temperature and can be derived from experimental measurements. The equation (27) allows calculating the time of complete droplet evaporation by assuming $d = 0$. Also the total mass flux of the fuel vapor coming from a single droplet can be determined as follows:

$$\dot{m}_v = \frac{\pi \cdot K \cdot d_0 \cdot \rho_f}{6} \tag{28}$$

where:

$\dot{m}_v$ –fuel vapor mass flux generated by evaporating single droplet of initial diameter d_0 [g/s],

ρ_f–fuel density [g/mm^3],

K, d_0–the same values as for equation (27).

The mass flux of fuel vapor coming from the entire spray jet depends on the numbers of droplets and their size distribution (atomization spectrum). Exact quantitative calculations are practically impossible here. Hence, the averaging equivalent values must be considered including droplet mean diameter and the number of droplets in accordance with actual fuel volume injected. From the droplet equivalent size theory we can estimate the number of

droplets of Sauter mean diameter $d_{3,2}$ covered by the spray jet consisting of the liquid fuel of a volume V_f:

$$x = \frac{6 \cdot V_f}{\pi \cdot d_{3,2}^3} \tag{29}$$

where:

x–the number of droplets of Sauter mean diameter $d_{3,2}$ inside the spray jet [–],

V_f–the volume of injected and atomized fuel [mm^3],

$d_{3,2}$–Sauter mean diameter (SMD) [mm].

The mass flux of fuel vapor that comes from the entire stream jet is calculated as follows:

$$\dot{M}_v = \dot{m}'_v \cdot x = \frac{\pi \cdot p_1 K \cdot d_{3,2} \cdot \rho_f}{6} \cdot \frac{6 \cdot V_f}{\pi \cdot d_{3,2}^3} = \frac{p_1 K \cdot \rho_f \cdot V_f}{d_{3,2}^2} \tag{30}$$

where:

$\dot{M}_v$ –total mass flux of fuel vapor [g/s],

$\dot{m}'_v$ –mass flux of fuel vapor comes from evaporation of single droplet located in a cloud of droplets [g/s],

x–the number of droplets in the stream jet [–],

p_1–factor correcting vaporization intensity of droplets (K) located in the cloud; typical value of p_1 is $p_1 \approx 0.8$-0.9,

K, d_{32}, V_f, ρ_f – the same values as for equations (27)-(29).

The value of p_1, according to (Kowalewicz & Mozer, 1977; Kucharska-Mozer, 1975; Mozer, 1976), respects the impact of cloud of droplets on the single evaporating droplet. It decreases the value of evaporation intensity factor K, because the close presence of other evaporating droplets slows down vaporization due to local temperature lowering.

Finally, it was assumed that the change of droplets size produces the same effect as the change of quantity of droplets of unchanged diameter. Then, the instantaneous fuel vaporization speed (total fuel vapor flux) can be expressed by differential equation:

$$\frac{dM_v}{d\varphi} = \frac{p_1 K\left(T_{II}(\varphi)\right) \cdot \rho_f \cdot V_f(\varphi)}{6 \cdot n \cdot d_{3,2}^2} \cdot 10^{-6} \tag{31}$$

where:

$dM_v/d\varphi$–instantaneous fuel vaporization speed [kg/deg],

φ–independent variable: the current crankshaft angle position [deg],

$K(T_{II}(\varphi))$–evaporation intensity factor as the function of the zone II temperature [mm^2/s],

n–crankshaft rotational speed [1/min],

$V_f(\varphi)$–instantaneous volume of liquid fuel in the stream jet [m^3],

–remaining denotations are as same as in equations (28)-(30).

Instantaneous volume of liquid fuel in the stream jet depends on fuel injection rate and fuel vaporization speed. It can be described by the following differential equation:

$$\frac{dV_f}{d\varphi} = \dot{V}_{inj}(\varphi) - \dot{V}_v(\varphi) = \dot{V}_{inj}(\varphi) - \frac{\dot{M}_v(\varphi)}{\rho_f} = \\ = \dot{V}_{inj}(\varphi) - \frac{p_1 K\left(T_{II}(\varphi)\right) \cdot V_f(\varphi)}{6 \cdot n \cdot d_{3,2}^2} \cdot 10^{-6} \tag{32}$$

where:

$dV_f/d\varphi$–change of liquid fuel volume in the stream jet [m^3/deg],

$\dot{V}_{inj}(\varphi)$ –volumetric fuel injection rate [m^3/deg],

–remaining denotations are as same as in equation (31).

By resolving equations (30) and (31) that are related each to other we get the rate of evaporated fuel as the function of crankshaft rotation angle. When the calculations exceed the moment of an autoignition, combustion will start and consequntly, the equation (31) will cover the additional component describing fuel vapor loss due to its burning.

3.4 Models for formation of chemical compounds

The chemistry of combustion and formation of different compounds can be included into the overall structure of the presented model. It will be shown on the example of NO formation, where the two of reversible Zeldovich's reactions will be analyzed (Zeldovich et. al., 1947, as cited in Heywood, 1988; Kafar & Piaseczny, 1998):

$$O + N_2 \leftrightarrow NO + N \tag{33}$$

$$N + O_2 \leftrightarrow NO + O \tag{34}$$

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

$$\frac{1}{V} \cdot \frac{dn_{NO}}{dt} = 2k_1 \cdot [O] \cdot [N_2] \tag{35}$$

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

$$[\mathrm{O}] = \left(K^c{}_{\mathrm{O}} \cdot [\mathrm{O}_2]\right)^{\frac{1}{2}} \tag{36}$$

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 (35) takes a following shape (all denotations are as same as above):

$$\frac{1}{V} \cdot \frac{dn_{\mathrm{NO}}}{dt} = 2k_1 \cdot K_{\mathrm{O}}^{c\,\frac{1}{2}} \cdot [\mathrm{O}_2]^{\frac{1}{2}} \cdot [\mathrm{N}_2] \tag{37}$$

The same formula can express a mass flux of NO in kilograms, so as to be used directly in the model differential equation system:

$$\frac{dM_{\mathrm{NO}}}{d\varphi} = \frac{\mu_{\mathrm{NO}} \cdot V}{6000 \cdot n} \cdot \left[2k_1 \cdot K^c{}_{\mathrm{O}}{}^{\frac{1}{2}} \cdot [\mathrm{O}_2]^{\frac{1}{2}} \cdot [\mathrm{N}_2] \right] \tag{38}$$

where:

μ_{NO}–molar mass of nitric oxide [g/mole]; μ_{NO} = 30.0061,

n–engine crankshaft 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 (Heywood, 1988; Rychter & Teodorczyk, 1990), and are equal to:

$$k_1 = 7{,}6 \cdot 10^7 \cdot \exp\left(\frac{-38000}{T}\right) \left[\frac{\mathrm{m}^3}{\mathrm{mole} \cdot \mathrm{s}}\right] \tag{39}$$

$$K^c{}_{\mathrm{O}} = \frac{10^{\left[\begin{array}{l} 5+0{,}310805 \cdot \ln(T) - \frac{12954}{T} + \\ +1{,}07083 - 0{,}738336 \cdot 10^{-4} \cdot T + \\ +0{,}344645 \cdot 10^{-8} \cdot T^2 \end{array}\right]}}{\bar{R}T} \left[\frac{\mathrm{mole}}{\mathrm{m}^3}\right] \tag{40}$$

4. Conclusion

The mathematical model of combustion that is presented in brief in this chapter consists of a lot of phenomena. Here, the most important like the energy conversion, fuel injection and NO_X formation are presented. Many of physical and chemical events occurred in the actual engine have been omitted in the model or considered in a reduced form. It is because of impossibility in their exact mathematical representation. Surely, it influences model accuracy, but can be partially compensated by pre-calculation parametric estimation process. This way of model validation shows the disadvantage, i.e. it has to be anew performed for each engine taken under simulation. Nevertheless, the presented model can be a valuable research tool to be used for extensive studies on combustion in all types of stratified charge engines.

5. References

Benson, R.S. & Whitehouse, N.D. (1979). *Internal Combustion Engines*. Pergamon Press, ISBN 978-008-0227-20-7, Oxford

Heywood, J.B. (1988). *Internal Combustion Engines Fundamentals*. McGraw Hill Co., ISBN 0-07-028637-X, New York, NY

Hiroyasu, H. & Kadota, T. (1976). Models for Combustion and Formation of Nitric Oxide and Soot in Direct Injection Diesel Engines. SAE Technical Paper 760129, *SAE Trans,* SAE Inc., Warrendale, PA

Kafar, I. & Piaseczny, L. (1998). Mathematical Model of Toxic Compound Emissions in Exhaust Gases Produced by Marine Engines. *Journal of KONES*, Vol.5, No.1, pp. 131-141, ISSN 1231-4005, Warsaw-Gdańsk, Poland

Khan, I.M., Greeves, G. & Wang C.H.T. (1973). Factors Affecting Smoke and Gaseous Emissions from Direct Injection Engines and a Method of Calculation. SAE Technical Paper 730169, *SAE Trans,* SAE Inc., Warrendale, PA

Kowalewicz, A. & Mozer, I. (1977). Method for cylinder pressure and temperature rate calculation in compression-ignition engine based on fuel injection characteristics (in Polish: Metoda określania przebiegu ciśnień i temperatur w cylindrze silnika wysokoprężnego na podstawie charakterystyki wtrysku). *5th International Simposium on Combustion Processes*, Cracow, Poland

Kowalewicz, A. (2000). *Fundamentals of Combustion Processes* (in Polish: Podstawy procesów spalania). WNT, ISBN 83-204-2496-8, Warsaw, Poland

Kucharska-Mozer, I. (1975). *Simulation of cylinder pressure and temperature in direct injection diesel engine based on fuel injection characteristics. Part I.* (In Polish: Metoda symulacji przebiegu temperatur i ciśnień w cylindrze silnika wysokoprężnego z wtryskiem bezpośrednim na podstawie charakterystyki wtrysku). Report No.3.41.113, Institute of Aviation, Warsaw, Poland

Kuszewski, H. & Szlachta, Z. (2002). Ecological point of fuel spray jet shaping in compression-ignition engine (in Polish: Ekologiczny aspekt kształtowania własności strugi rozpylanego paliwa w silniku wysokoprężnym). *Problemy Eksploatacji*, No.1, pp. 163-173, ITE, Radom, Poland

Mozer, I. (1976). *Simulation of cylinder pressure and temperature in direct injection diesel engine based on fuel injection characteristics. Part II.* (In Polish: Metoda symulacji przebiegu temperatur i ciśnień w cylindrze silnika wysokoprężnego z wtryskiem

bezpośrednim na podstawie charakterystyki wtrysku - część II: Symulacja cyfrowa). Report No.3.41.1.6, Institute of Aviation, Warsaw, Poland

Orzechowski, Z. & Prywer, J. (1991). *Spraying liquids* (in Polish: Rozpylanie cieczy). WNT, ISBN 83-204-1378-8, Warsaw, Poland

Patterson, M.A.; Kong, S.C.; Hampson, G.J. & Reitz, R.D. (1994). Modeling the Effects of Fuel Injection Characteristics on Diesel Engine Soot and NO_X Emissions. SAE Technical Paper 940523, *SAE Trans,* SAE Inc., Warrendale, PA

Patterson, M.A. (1997). *Modeling the Effects of Fuel Injection Characteristics on Diesel Combustion and Emissions*. Ph.D. Thesis, University of Wisconsin-Madison

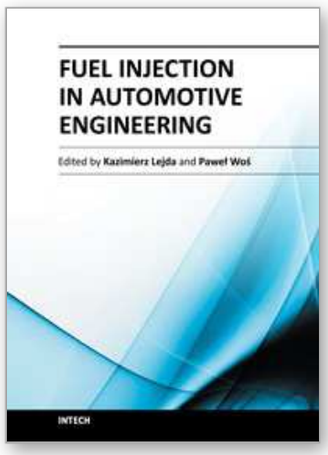
Rychter, T. & Teodorczyk, A. (1990). *Mathematical Modeling of Piston Engine Working Cycle* (in Polish: Modelowanie matematyczne roboczego cyklu silnika tłokowego). PWN, ISBN 978-830-1096-42-7, Warsaw 1990,.

Shaded, S.M.; Chiu, W.S. & Yumlu, V.S. (1973). A Preliminary Model for the Formation of Nitric Oxide in Direct Injection Diesel Engines and Its Application in Parametric Studies. SAE Technical Paper 730083, *SAE Trans,* SAE Inc., Warrendale, PA

Wajand, J.A. (1988). *Compression ignition engines* (in Polish: Silniki o zapłonie samoczynnym), WNT, ISBN 978-832-0401-68-4, Warsaw, Poland

Woś, P. (2008). *Effect of Fuel Injection Rate on Combustion and NO_X Emission in Diesel Engine. Mathematical approach* (in Polish: Wpływ przebiegu wtrysku paliwa w silniku wysokoprężnym na spalanie i emisję NO_X). Rzeszów University of Technology, ISBN 978-83-7199-519-4, Rzeszów, Poland

Zabłocki, M. (1976). Fuel Injection and Combustion in Diesel Engines (in Polish: Wtrysk i spalanie paliwa w silnikach wysokoprężnych). WKŁ, Warsaw, Poland



Fuel Injection in Automotive Engineering

Edited by Prof Kazimierz Lejda

ISBN 978-953-51-0528-2
Hard cover, 144 pages
Publisher InTech
Published online 20, April, 2012
Published in print edition April, 2012

The main topic of "Fuel injection in automotive engineering" book is fundamental process that determines the development of internal combustion engines and performances of automotive vehicles. The book collects original works focused on up-to-date issues relevant to improving injection phenomena per se and injection systems as the engine key components.

How to reference

In order to correctly reference this scholarly work, feel free to copy and paste the following:

Kazimierz Lejda and Paweł Woś (2012). Simulation of Combustion Process in Direct Injection Diesel Engine Based on Fuel Injection Characteristics, Fuel Injection in Automotive Engineering, Prof Kazimierz Lejda (Ed.), ISBN: 978-953-51-0528-2, InTech, Available from: http://www.intechopen.com/books/fuel-injection-in-automotive-engineering/simulation-of-combustion-process-in-direct-injection-diesel-engine-based-on-fuel-injection-character

INTECH
open science | open minds

InTech Europe
University Campus STeP Ri
Slavka Krautzeka 83/A
51000 Rijeka, Croatia
Phone: +385 (51) 770 447
Fax: +385 (51) 686 166
www.intechopen.com

InTech China
Unit 405, Office Block, Hotel Equatorial Shanghai
No.65, Yan An Road (West), Shanghai, 200040, China
中国上海市延安西路65号上海国际贵都大饭店办公楼405单元
Phone: +86-21-62489820
Fax: +86-21-62489821

IntechOpen