

Multi-Zone DI Diesel Spray Combustion Model for Thermodynamic Simulation of Engine with PCCI and High EGR Level

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ABSTRACT

A multi-zone, direct-injection (DI) diesel combustion model, the so-called RK-model, has been developed and implemented in a full cycle simulation of a turbocharged engine. The combustion model takes into account:

- transient evolution of fuel sprays,
- interaction of sprays with swirl and walls,
- evolution of near-wall flow formed after spray-wall impingement depending on impingement angle and local swirl velocity,
- interaction of Near-Wall Flows (NWF) formed by adjacent sprays,
- influence of temperatures of gas and walls in the zones on evaporation rate.

In the model the fuel spray is split into a number of specific zones with different evaporation conditions including zone on the cylinder liner and on the cylinder head. The piston bowl is assumed to be a body of revolution with arbitrary shape. The combustion model supports central and non-central injector as well as the side injection system. NO_x formation model uses Detail Kinetic Mechanism (199 reactions with 33 species). Soot formation model is phenomenological. The general equation for prediction of ignition delay period was derived as for conventional engines as for engines with PCCI where pilot injection timing achieved 130 CA deg. before TDC. The model has been validated by experimental data obtained from high-speed, medium-speed and low-speed engines over the whole operating range; a good agreement has been achieved without recalibration of the model for different operating modes. General equations for prediction of spray tip penetration, spray angle and ignition delay for low temperature

combustion and high temperature combustion were derived and validated with the published data obtained for different diesels including diesels with multiple injection system and injection timing varied from very early up to after the TDC.

To make a computational optimization of multiple injection strategy possible, the full cycle thermodynamic engine simulation software DIESEL-RK has been supplied with library of nonlinear optimization procedures.

INTRODUCTION

The combustion process as well as NO_x and PM emissions formation in direct-injection diesels are very sensitive to engine parameters such as the sprayer design and location, the piston bowl shape, swirl intensity, strategy of EGR use, and injection profile including multiple electronic controlled injection.

One area that still holds potential for lowering NO_x emissions within the engine is the modification of the combustion process so that more of the combustion occurs under lean conditions, which reduces local combustion temperatures and NO_x formation. Lowering combustion temperature allows simultaneously reduce NO_x and soot formation. One method of achieving overall lean combustion is Premixed Charge Compression Ignition (PCCI) or Homogeneous Charge Compression Ignition (HCCI) where the entire fuel and air charge is premixed prior to the start of combustion. PCCI/HCCI has been the focus of numerous researches due to its potential for extremely low NO_x without increases in PM or fuel consumption. Due to the high rate of pressure rise and problems with controlled start of combustion there are challenges of use the

PCCI/HCCI operation over the full engine operating range. So at computational analysis of an engine the mathematical model and computer code have to support both the conventional engine combustion and PCCI/HCCI combustion without discontinuity to make it possible the computer optimization of engine control parameters over the whole engine operating range.

Due to a great number of available options and their combinations, a search for the optimal solution is a long and labor-consuming task. Simulation as well as computational optimization can effectively point out trends and effective ways of engine improvement.

There are nowadays three categories of diesel engine simulation models:

- Zero-dimensional single-zone models;
- Quasi-dimensional multi-zone models;
- Multi-dimensional models (CFD).

Although CFD possesses, in principle, the ability to simulate all fluid-flow/heat-transfer/chemical-reaction phenomena, in practice it is limited by: a) the limited capability of current computers to handle small-scale phenomena in an acceptably short time; b) the inadequacy of current scientific knowledge about turbulence, two-phase flow and chemical reaction, especially when all three are simultaneously presented. So, the attempt to optimize diesel-engine processes by way of 'pure CFD' cannot be succeeded at present.

The choice of the thermodynamic engine model together with quasi-dimensional multi-zone model of combustion accounting peculiarities of conventional and PCCI diesel combustion is conditioned by requirements of high accuracy and the high computational speed, because the number of engine simulation sessions in optimization over the whole operating range comes up to few thousands.

The earlier published multi-zone diesel spray combustion model [1, 2, 3], named the RK-model includes three independent emission submodels: the NO_x formation submodel based on the Zeldovich's scheme [4] developed by Zvonov [5]; the soot formation submodel developed by Razleytsev [6]; the advanced NO_x formation submodel based on Detail Kinetic Mechanism (DKM) for correct prediction of NO emission in engine with large EGR, multiple injection and PCCI/HCCI. DKM includes 199 reactions with 33 species, one was built on the kinetic scheme by prof. Basevich V.J. [5, 7, 8, 9]. Soot and NO_x formation processes are simulated with separate procedures after combustion modeling. The main equations of the RK-model were derived by Razleytsev in 1990-1994. This method afterwards was modified and complemented by Kuleshov [1, 2, 3].

The RK-model takes into account conditions of evolution of each fuel spray and near-wall flows generated by sprays; and also interaction between sprays and swirl, as well as between near-wall flows, formed by adjacent

sprays. These features of the RK-model allow prediction of diesel combustion and emissions over the whole operating range for the following varying parameters:

- piston bowl shape and sprayer location;
- swirl intensity;
- number, diameter and direction of sprayer nozzles;
- injection profile shape and any multiple injection.

A more detailed description of the RK-model was given in [1, 2, 3, 53]. The present paper describes the same model with peculiarities being implemented to improve accuracy of heat release prediction in diesels with PCCI.

GENERAL PRINCIPLES OF SPRAY MODELLING

The theoretical background of the model is based on the method developed in [6] in which the fuel spray injected into the combustion chamber of the engine is split into a number of specific zones. This is caused by the necessity of detailed account for following fuel spray evolution peculiarities:

- difference of fuel droplet evaporation conditions in different spray zones;
- fuel redistribution among zones in the process of free spray movement and in its interaction with a wall;
- interaction of fuel sprays with the walls of the piston bowl and possibility of fuel hitting the cylinder liner and the cylinder head surface;
- effect of the wall temperature on the fuel evaporation rate in near-wall zones;
- interaction of adjacent sprays in near-wall flows.

The spray evolution passes through three stages:

- Initial formation of dense axial flow.
- Main stage of cumulative spray evolution.
- Period of spray interaction with the combustion chamber walls and fuel distribution on the walls.

Liquid spray breakup takes place close to the nozzle. High-speed fuel portions move quickly towards the spray tip pushing apart, impacting and thus coalescing with droplets formed earlier. In the spray cross section the distribution density of droplets and their diameter reduce rapidly with growing distance from the spray axis. In this context, near the jet boundary droplets are slowed down more rapidly than those near the axis and are gradually delayed and separated from them.

At the main evolution stage later on, the axial flow is slowed down and concentrated on the forward front side because of the surrounding gas resistance. New flying fuel portions reach the axial flow, penetrate inside, push and condense it at the rear. This results in an extended axial core with increased density and droplet velocity being formed in the middle of the spray [10]. This core is surrounded by a relatively dilute outer sleeve made of delayed droplets. Corresponded scheme of diesel fuel spray is presented in Fig. 1.



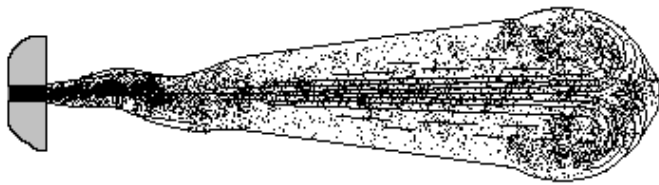


Figure 1. Scheme of diesel fuel spray, concentration of fuel droplets and its tracks.

The border between the initial and main stages of spray evolution corresponds to the moment when the axial flow close to the spray tip starts to deform and break up, forming a condensed mushroom-shaped forward front. As the spray moves on, constant breakup of the spray forward part [11] takes place and the front is renewed by new flying fuel portions [12, 13]. The delayed droplets move from the breaking front to the environment. The moving spray carries the surrounding gas with it, the gas velocity in the environment being rather low. Meanwhile gas in the axial core is rapidly accelerated to the velocity close to that of droplets [14]. The core diameter in the cross section is about 0.3 of the spray outside diameter.

In accordance with [6], the current position and the velocity of an Elementary Fuel Mass (EFM) injected during small time-step and moving from the injector to the spray tip are related as

$$\left(\frac{U}{U_o} \right)^{\frac{3}{2}} = 1 - \frac{l}{l_m} \quad (1)$$

where: l is the current distance between the injector's nozzle and the EFM; $U = dl/d\tau_k$ is the current velocity of the EFM; τ_k is the travel time for the EFM to reach a distance l from the injector's nozzle; U_o is the initial velocity of the EFM at the nozzle of the injector and l_m is the EFM's penetration distance.

As an illustration, Fig. 2 presents the variation of spray evolution parameters l , l_m , U and U_m as functions of time for a medium speed diesel engine.

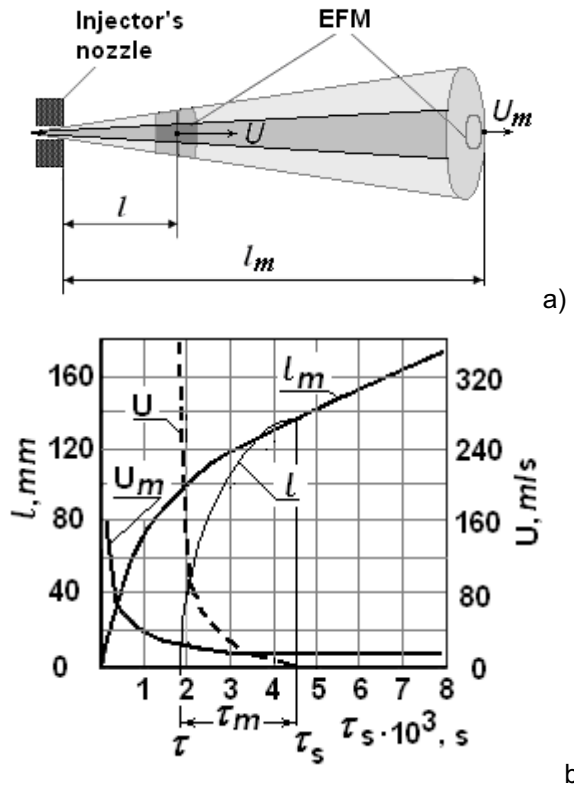


Figure 2. The simplified sketch of the spray (a) and variations of spray evolution parameters: l , l_m , U and U_m as functions of time (b).

Upon termination of fuel evolution there is still some fuel in its axial core supplied at the final injection stage. At the initial combustion stage the flame is unable to break up the fuel spray condensed core [15, 16, 6] which explains why the sprays continue to move to the combustion chamber sidewalls during injection even after fuel ignition. By the end of fuel supply a considerable fraction of the fuel cycle portion is accumulated near the walls. This takes place both in diesels with compact combustion chambers and in engines with wide piston bowls (Hesselman). The interaction of fuel sprays with chamber walls was studied in numerous literature sources [17-24]. Having analyzed various data, Razleytsev proposed the following model of fuel spray interaction with a wall. On reaching the wall, the spray is spread over its surface in every direction. The upward flow over the wall gets quickly into a clearance between the piston and cylinder head and under constricted conditions spreads along the piston crown as well as the cylinder head surface (Fig. 3). A part of fuel can reach the cylinder liner. Analysis of experimental data has shown that characteristics of flows moving along the wall in different directions are similar to those obtained for a freely moving spray, but the velocity level is lower and depends on the flow direction. Reduction in the flow velocity along the wall is

caused by the hydrodynamic resistance of the nearby wall.

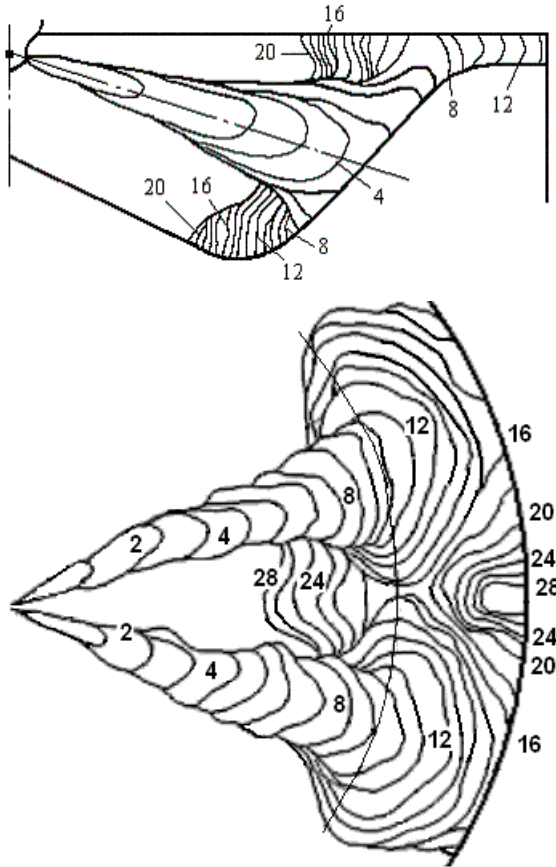


Figure 3. Photo-record obtained by Koptev, Gavrilov [25], Plotnikov. Fuel was injected into the bomb with the piston model. Nozzles: 7 x 0.4 mm. Speed of shooting is 3700 frame/sec. The numbers correspond to frames of shooting.

The mentioned similarity in evolution between near-wall flows and free sprays provides the basis for the application of the same computational procedures to near-wall flows and free sprays. The assumption that the velocity of an elementary fuel portion flying along the wall is analogous to the fuel outflow velocity from a sprayer makes it possible to apply conventional criterion relations for simulation of the flows in the near-wall zone.

As the spray hits the wall, the forward front fuel enters the near-wall flow zone. The spray trajectory and, therefore, the time, the place and wall impingement angle are determined in view of the swirl effect. The process of spray interaction with a wall is rather complicated. The following scheme of spray and NWF evolution is proposed.

- During the spray forward front impingement with a wall a conical condensed gas-fuel layer is being formed there within the borders of a stain formed at the intersection of a conical spray with the wall surface (zone 4 in the fig. 10).

- On fast fuel spray front impingement with the wall the fuel spreads out of the initial stain limits.
- The high-speed axial flow of a spray in its hitting the wall thickens the near-wall layer, draws apart its borders and a part of the flow moves to its periphery above this layer.
- The shape of the near-wall stain and its spreading rate in various directions depend on the spray-with-the wall impingement angle and the air swirl effect.

A typical photo-record of the evolution of a spray in the combustion chamber is shown in Fig.3.

The partial solution of the differential equation 1 is:

$$3l_m \left[1 - \left(1 - \frac{l}{l_m} \right)^{0.333} \right] - U_0 \tau_k = 0 \quad (2)$$

where τ_k is the time of EFM movement from the nozzle up to l . When EFM is stopped in a spray tip $l = l_m$, $\tau_k = \tau_m$ and

$$l_m = U_0 \tau_m / 3. \quad (3)$$

From equations 1, 2, 3 it follows:

$$U = U_0 (1 - \tau_k / \tau_m)^2; \quad (4)$$

$$l = l_m \left[1 - (1 - \tau_k / \tau_m)^3 \right]. \quad (5)$$

Parameters of the spray tip are calculated with empirical equations of Lyshevsky [26]. These relations use dimensionless criteria:

$$We = U_{0m}^2 d_n \rho_f / \sigma_f; \quad (6)$$

$$M = Oh^2 = \mu_f^2 / (\rho_f d_n \sigma_f); \quad (7)$$

$$\Theta = \tau_s^2 \sigma_f / (\rho_f d_n^3); \quad (8)$$

$$\rho = \rho_{air} / \rho_f \quad (9)$$

where: U_{0m} is the average injection velocity, d_n is the nozzle hole diameter, ρ_f is the fuel density, ρ_{air} is the air density, σ_f is the fuel surface density, μ_f is the dynamic viscosity coefficient of fuel, τ_s is the current time from the injection beginning.

Evolution of a free spray consists of two main phases: a) initial phase of pulsing evolution; b) basic phase of cumulative evolution. The border between these phases is marked as l_g (length) and τ_g (time):

$$l_g = C_s d_n We^{0.25} M^{0.4} \rho^{-0.6}; \quad (10)$$

$$\tau_g = l_g^2 / B_s; \quad (11)$$

$$B_s = d_n U_{0m} We^{0.21} M^{0.16} / (D_s \sqrt{2} \rho); \quad (12)$$

where $C_s = 8.25 \div 8.85$; $D_s = 4.5 \div 5$ for diesel cylinder conditions. The spray tip penetration length in the initial (index a) and the base (index b) phases is calculated by the following empirical expressions [6]:

$$l_a = A_s \vartheta_g^{0.35} \exp[-0.2(\tau_s/\tau_g)]; \quad (13)$$

$$l_b = B_s^{0.5} \tau_s^{0.5}; \quad (14)$$

where: $A_s = 1.22 l_g \vartheta_g^{-0.35}$ and criterion ϑ_g are calculated by equation (8) with the assumption $\tau_s = \tau_g$. The form of equation (14) is close to that derived by Kuo [27] and Hiroyasu [28]. Equations (6-14) with $D_s = \text{const}$ were obtained by Lyshevsky for medium-speed diesels. To make this model suitable for high-speed diesels with small injector nozzles as well, the following expression for D_s was derived in the current investigation:

$$D_s = 14.21 / D_f \quad (15)$$

where:

$$D_f = \begin{cases} 2.9, & \text{if } d_n \geq 0.3 \\ 2.9(a \cdot d_n^3 + b \cdot d_n^2 + c \cdot d_n + d), & \text{if } d_n < 0.3 \end{cases}; \quad (16)$$

d_n is the nozzle diameter in millimeters; $a=9.749$; $b=7.45$; $c=-7.21$; $d=2.224$. Equations (15) and (16) have been derived as a result of analysis of experimental data on the dependence of a fuel spray penetration distance

from the value of the nozzle diameter and injection pressure published in [29–32]. In these investigations the diameter of the nozzles and injection pressures were varied from 0.11 to 0.45 mm and from 300 to 1200 bar, respectively. The results of this analysis demonstrate that the pressure of the fuel injection does not affect the value of D_s significantly. The variation of D_s as a function of d_n is shown in Fig.4.

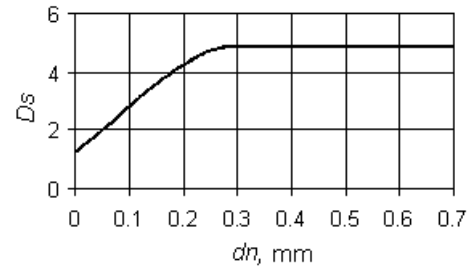


Figure 4. The variation of D_s as function of nozzle diameter d_n .

Comparison between calculated and measured spray tip penetrations for engines with different nozzles hole diameters d_n and different injection pressure values P_{inj} are shown in the Fig.5.

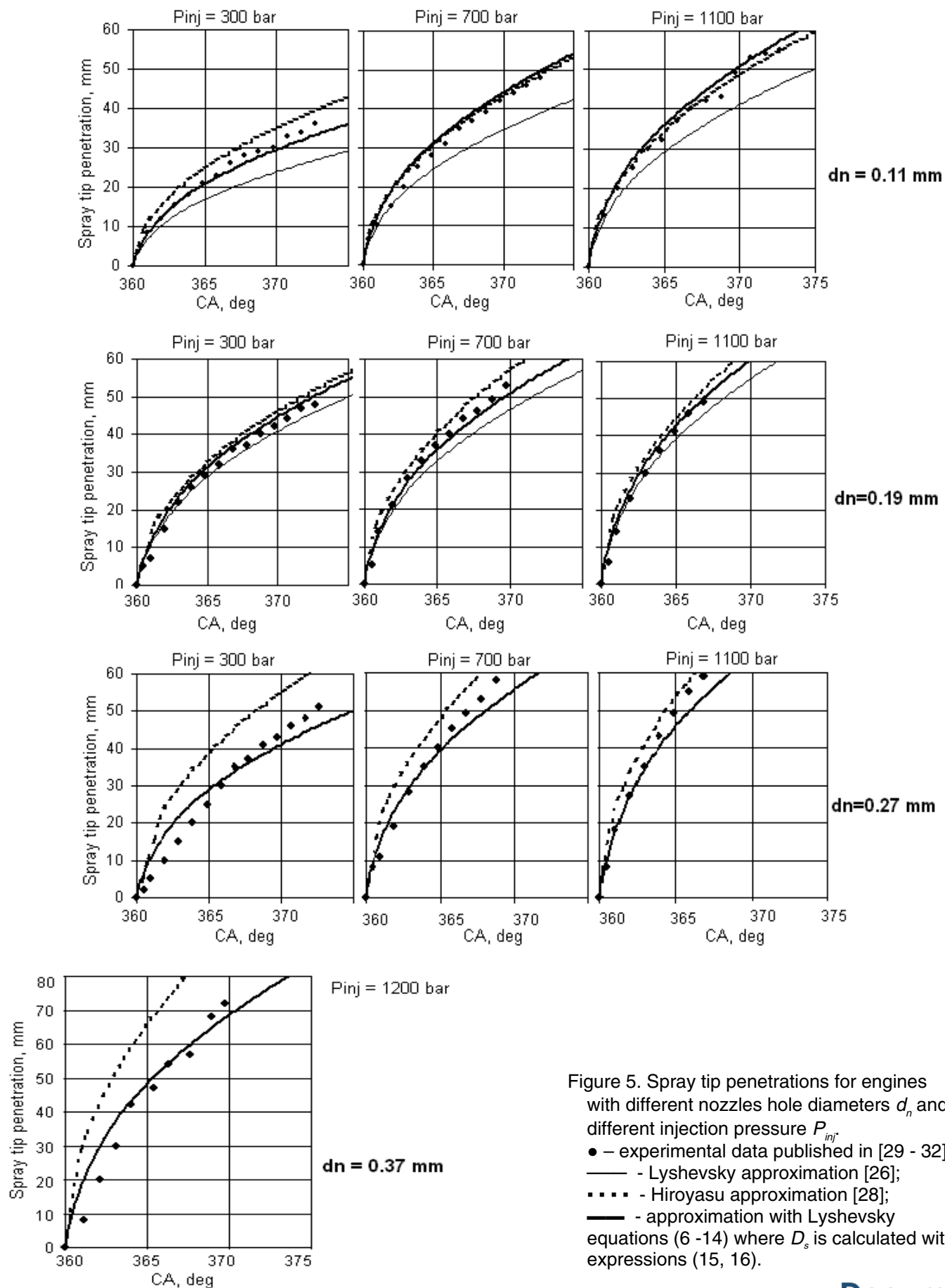


Figure 5. Spray tip penetrations for engines with different nozzles hole diameters d_n and different injection pressure P_{inj} .
 • – experimental data published in [29 - 32];
 — - Lyshevsky approximation [26];
 - Hiroyasu approximation [28];
 — - approximation with Lyshevsky equations (6 - 14) where D_s is calculated with expressions (15, 16).

Presented data show the Hiroyasu approximation is working well at small injector nozzle diameter ($d_n < 0.25$ mm), as well the Lyshevsky approximation [26] gives underrated spray tip penetration at small nozzles diameter. If nozzles diameter exceed 0.25 mm the Hiroyasu approximation overrates spray tip penetration, but the Lyshevsky approximation becomes to be working well. The presented equations (6-16) are general and show correct results over the wide range of spray nozzles diameter variation and at different injection pressures.

The spray angle is calculated as follows:

$$\gamma_a = 2 \operatorname{Arctg} \left(E_s We^{0.35} M^{-0.07} \mathfrak{D}^{-0.12} \rho^{0.5} e^{0.07 \tau_s / \tau_g} \right); \quad (17)$$

$$\gamma_b = 2 \operatorname{Arctg} \left(F_s We^{0.32} M^{-0.07} \mathfrak{D}^{-0.12} \rho^{0.5} \right) \quad (18)$$

where: $E_s = 0.932 F_s We^{-0.03} \mathfrak{D}^{0.12}$ and criterion $\mathfrak{D}_g$ are calculated by equation (8) with the assumption $\tau_s = \tau_g$, $F_s = 0.0075 \div 0.009$ for diesel cylinder conditions. The free spray contour angles obtained by different simulation methods and experimentally are compared in Fig. 6.

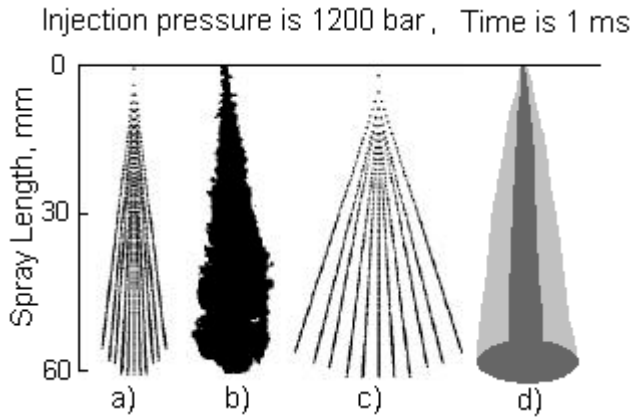


Figure 6. The free spray contours obtained by different ways: a) calculated with KIVA by Reitz and Bracco [33]; b) measured by Dan [34]; c) calculated by Jung and Assanis [35] using Hiroyasu and Arai equations [36]; d) calculated with equations (17, 18).

If a swirl with angular velocity ω exists in the combustion chamber then the spray is deformed and deflected by some distance y in the tangential direction inside the chamber, as shown in Fig. 7. The deformation of the initial conical form of the spray is characterized by the parameters y , y_3 , y_4 and r . Local tangential air velocity is:

$$W_t = \chi R_s \pi n R / 30; \quad (19)$$

where: $R_s = \omega / \omega_c$ is the swirl ratio, n is the engine speed, R is the current radius, χ is the swirl damping factor depending on CA. Tangential velocity of EFM in

the swirl direction U_t is defined by the equation published in [37]:

$$dU_t / d\tau = A_{wt} W_t^{1.5}; \quad A_{wt} = 0.75 C \rho \nu^{0.5} d_{32}^{-1.5} \quad (20)$$

where: $C \approx 5$ is empirical coefficient, ν is air viscosity, $d_{32} = 1.7 d_n M^{0.0733} (We \rho)^{-0.266}$ is Sauter Mean Diameter of drops. The deflection distance of the spray axis at each time step due to swirl is: $\Delta y = U_t \Delta \tau \cos \beta$, where: $\Delta \tau$ is time step, β is an angle between radius and current sector of axis. Deformation by swirl of windward Δy_3 and leeward Δy_4 generating lines of the spray core cross section are calculated for each time step as:

$$\begin{aligned} dy_3 &= -C_{30} A_{wt} (W_t - U_t) \Delta \tau \cos \beta; \\ dy_4 &= C_{40} A_{wt} (W_t - U_t) \Delta \tau \cos \beta \end{aligned} \quad (21)$$

where: $C_{30} \approx 0.2$ and $C_{40} \approx 1.6$ are empirical coefficients.

After wall impingement a dense near-wall flow consisting of fuel drops and air, arises. The NWF expands on a surface in all directions. The shape of NWF spot depends on impingement angles: γ_j ($j = 1, 2, 3, 4$) (see Fig. 7).

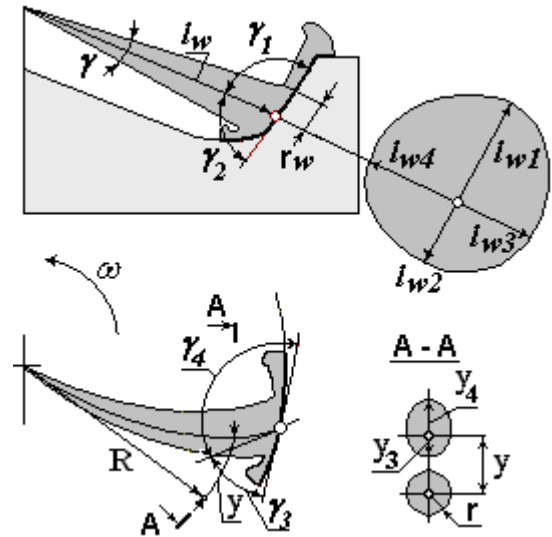


Figure 7. Schematic of a spray and near-wall flow in swirling air.

Impingement angles are calculated with allowance for swirl transfer of a spray and the shape of a piston bowl in a place of impingement. Dimensions of NWF spot in each directions l_{wj} ($j = 1, 2, 3, 4$) are defined as follows:

$$\begin{aligned} l_{wj} &= K_j B_{sw}^{0.5} \tau_w^{0.5}; \quad \tau_w = \tau_s - \tau_{sw}; \\ B_{sw} &= \left[(\phi + 0.08 K_{j \max}) / K_{j \max} (l_{b \max} - l_w) \right]^2 / (\tau_{s \max} - \tau_{sw}) \end{aligned} \quad (22)$$

where: $\phi = 0.6$ is the factor of losses due to impingement, τ_{sw} is the time of impingement¹, $\tau_{s\max} = \tau_{inj} + (0.3 \div 0.5)10^{-3}$ [s] is the time of complete spray evolution, $l_{b\max}$ is a free spray length in complete evolution, l_w is the distance covered by a spray before impingement.

On the basis of experimental photo-records made by Gavrilov, Koptev, and Plotnikov the following expression for NWF spot dimensions versus impingement angles $\gamma_1, \gamma_2, \gamma_3, \gamma_4$, (fig. 7) was derived by Gavrilov [25]:

$$K_j = \sqrt{\sin \gamma_1 \sin \gamma_3} + 1.2(1 - \sin \gamma_j) - 2(\cos \gamma_j)^3; \quad (23)$$

$$K_{j\max} = \text{MAX}(K_1, K_2, K_3, K_4).$$

The time of wall impingement τ_{sw} is determined by the equations (13, 14, 20) with account for spray tip 3-D coordinates and piston movement.

Comparison of calculations of the spray tip penetration and NWF borders evolution by equations (6-23) with the experiment is shown in Fig. 8. The measured values are marked with points, frame numbers correspond to those in Fig. 3. Subscript "free" means free spray evolution (without walls).

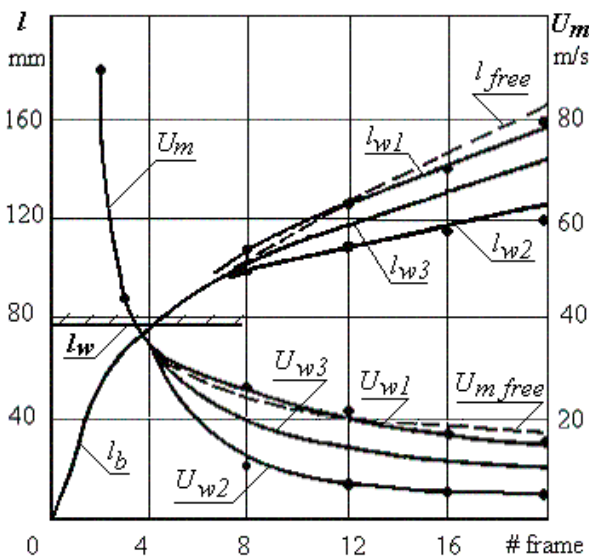


Figure. 8. Spray evolution phenomena in conditions of turbocharged diesel: S/D=300/230, RPM=750, $m_f = 0.62$ g. U_{wj} are velocities of corresponded NWF borders. Data was obtained by Razleytsev [6].

¹ Actually the wall impingement starts from the moment of spray front contact with an oblique surface of the piston and is completed by full transition of fuel from the front in the core of NWF. Due to schematic description of RK-model in this paper, this algorithm is skipped here.

For visualization of fuel spray evolution a special Fuel Spray Visualization (FSV) computer code has been developed. Spray images presented below are obtained with this code. Comparison of the calculated image of spray and NWF evolution with the experimental photo-record is presented in Fig. 9. Frame "b" shows pictures of near-wall flows obtained by superposition of shooting frames with the sprays images artificially removed. The shapes of the NWF spots experimentally obtained agree with the calculated ones.

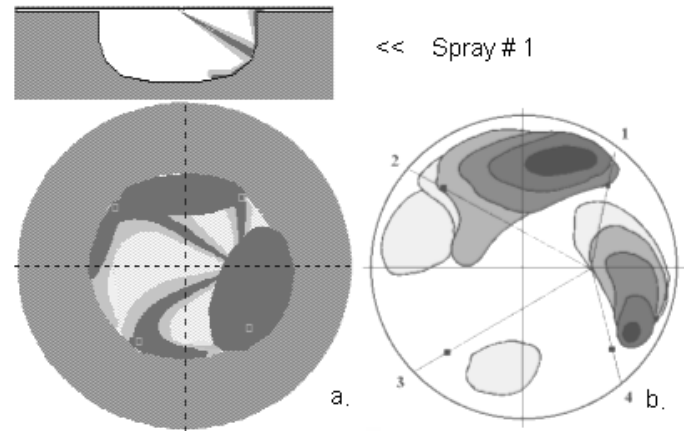


Figure 9. Comparison of calculated image of spray and NWF evolution (a) with experimental photo-record (b) of tractor diesel: S/D =140/120, RPM=1800.

DISTRIBUTION OF FUEL IN A SPRAY

The principles of simulation of fuel distribution in a spray used in the RK-model were derived by Razleytsev [6]. A spray, which is injected into the combustion chamber, is divided into 7 characteristic zones as shown in Fig. 10. Each zone has own conditions of evaporation and burning and these conditions are uniform within a whole zone.

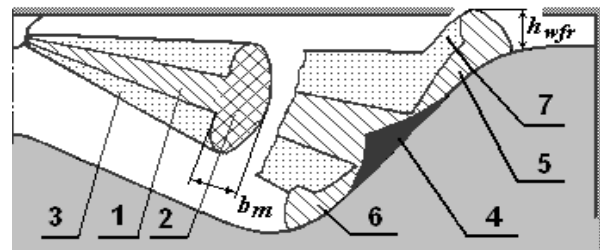


Figure 10. Characteristic zones of the diesel spray.

During the time prior to the jet impingement only three zones are considered in the spray. These are: 1 - dense conical core, 2 - dense forward front, 3 - dilute outer sleeve. The near-wall flow being formed after impingement is inhomogeneous in structure, density and temperature, which makes the calculation of the