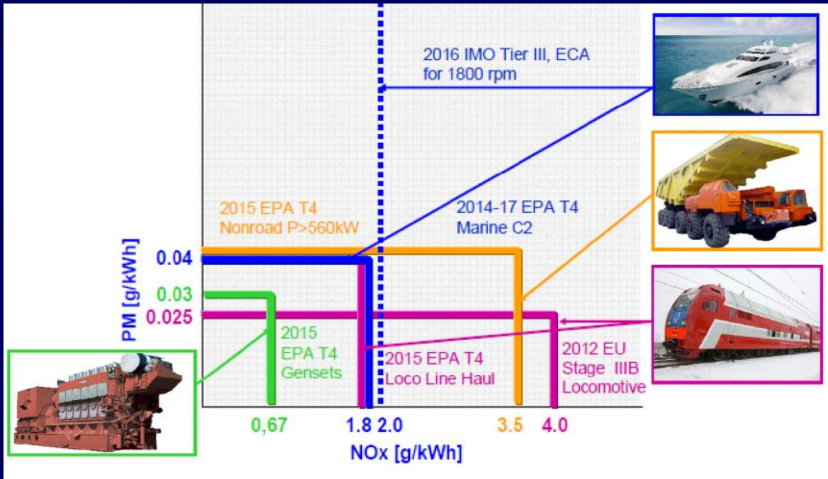
# DIESEL - RK

*Engine Simulation & Optimization Software*

# Thermodynamic engine simulation tools

The thermodynamic engine simulation tools are most applicable for general engine analysis and they are widely used because do not require large resources.

How to use them for diesel combustion optimization to meet emission regulations?




Gasexchange model ⇩ Combustion model ⇩

| | | |
|---|---|---|
| GT-Power<br>(Gamma Technology) | 1D | Wiebe; User model; Link with CFD;<br>DI Jet model (Hiroyasu). |
| BOOST<br>(AVL) | 1D | Wiebe; User model; Link with CFD;<br>Mix Control Combust (MCC) model. |
| AMESim<br>(LMS International) | 1D | Wiebe; User model; Link with CFD;<br>Mix Control Combust (MCC) model. |
| WAVE<br>(Ricardo) | 1D | Wiebe; User model; Link with CFD;<br>Hiroyasu. |
| DIESEL-RK | 1D | Wiebe; ***RK-Model*** |
| | | |

Standard tool

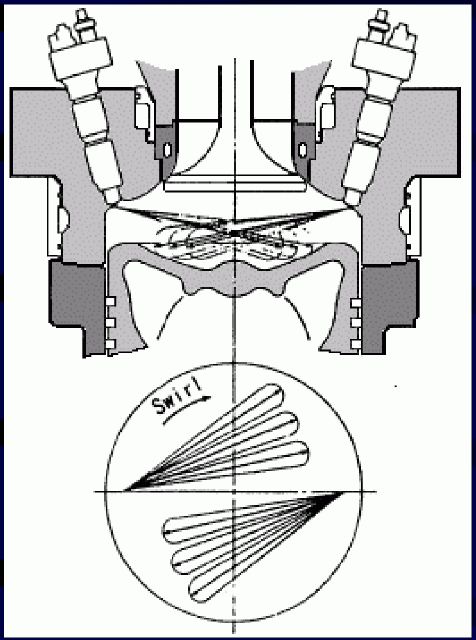
NO Combustion Optimization

Fast simulation + Optimization of Combustion

# Performance of Diesel Combustion Models

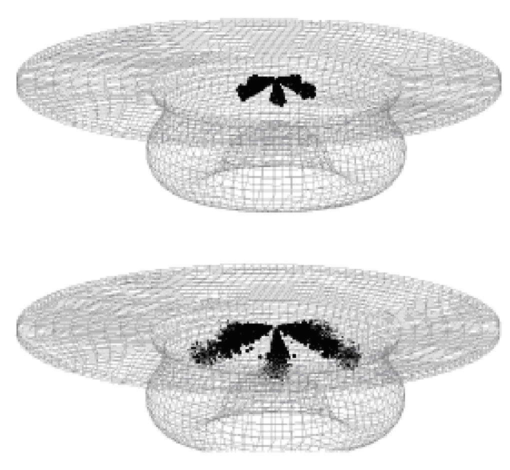
- Multi-Dimensional (CFD)

Require too much computational time
Formal optimization is not possible.




Time: 2 days

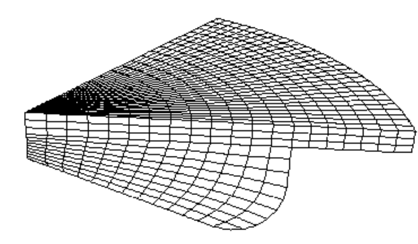
A



Time: 10 hours

B

From IVC till EVO

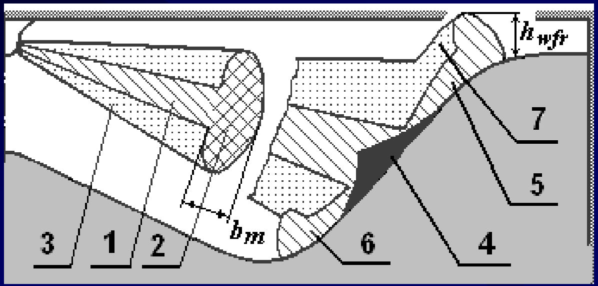


Time: 2 hours

C

- Quasi-Dimensional, Multi-zone ***RK-Model***

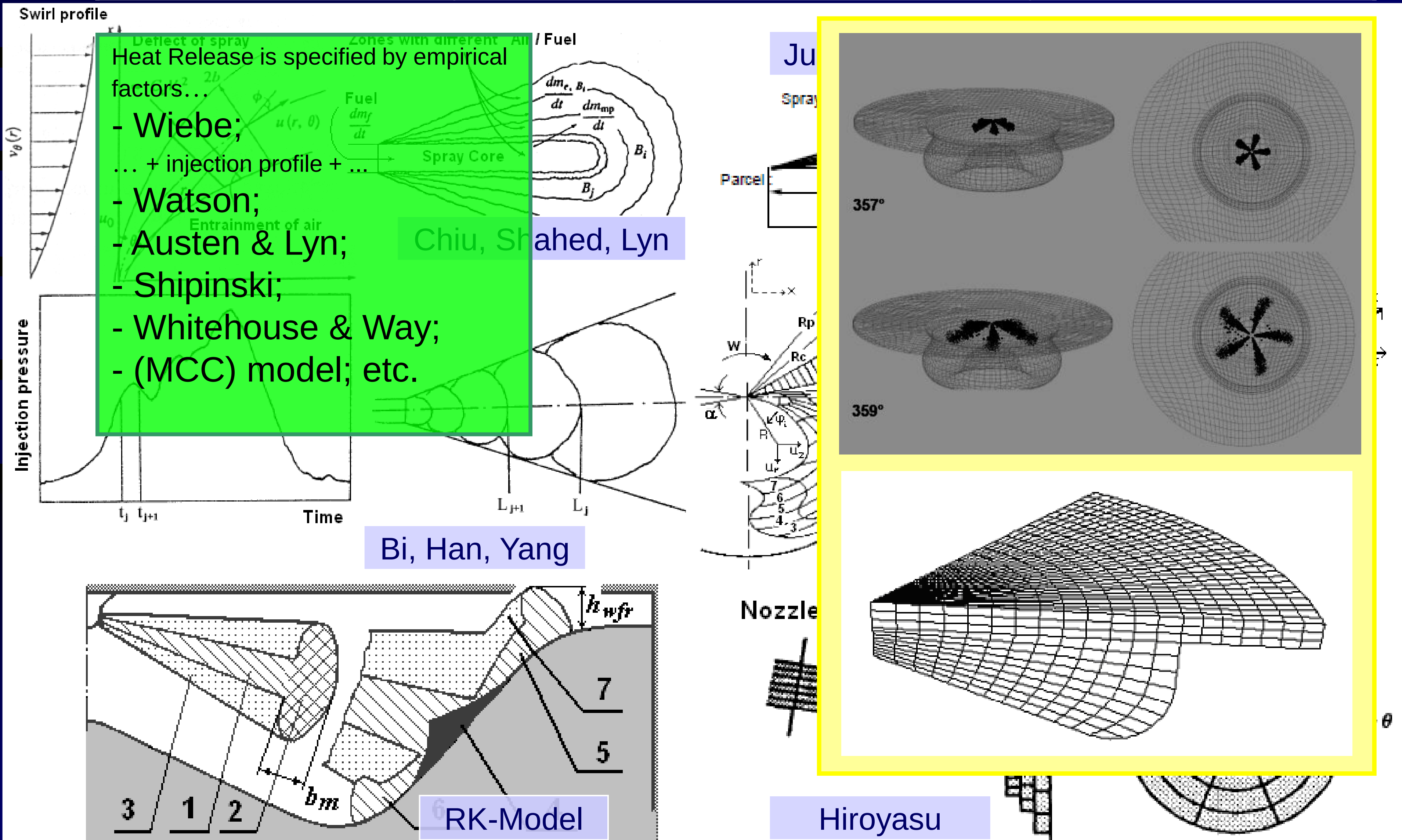
Time: 30 seconds instead of 4 days in case A




11 Zones of Spray

# Diesel combustion models

| Zero-dimensional, Single-zone | Quasi-dimensional, Multi-zone | Multi-Dimensional (CFD) |
|---|---|---|




Heat Release is specified by empirical factors…
- Wiebe;

… + injection profile + …
- Watson;
- Austen & Lyn;
- Shipinski;
- Whitehouse & Way;
- (MCC) model; etc.

Chiu, Shahed, Lyn

Bi, Han, Yang

RK-Model

Hiroyasu

# Workability of Diesel combustion models for engineering tasks of emission control

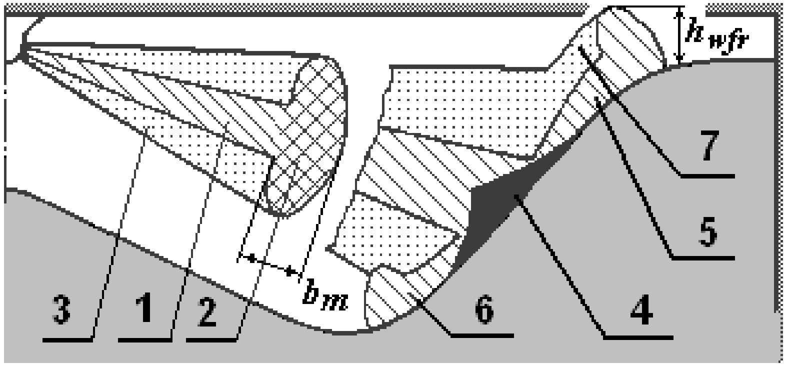
| Zero-Dimensional, Single-zone | Quasi-dimensional, Multi-zone | Multi-Dimensional (CFD) |
|---|---|---|
| **No, due to insufficient capabilities** | May be acceptable, if improved | **Require too much resources** |

Even the most advanced **Hiroyasu model** has failings:
- Does not account piston motion;
- Supports only easy shapes of piston bowls;
- Supports only central location of injector;
- Does not account interaction among sprays;
- Does not account mass-exchange among packages;
- Does not account hitting of fuel on cylinder liner and head.

The existing Quasi-dimensional multi-zone models have limitations at resolving combustion optimization tasks due to
- Insufficiently detailed consideration of determining processes of mixture formation, combustion, emission formation;
- as a result they have Insufficient accuracy of simulation of combustion and emission.

**So, the most actual problems of engine simulation and their optimization are out of capabilities of existing simulation tools**

**We offer to use an another concept of Multi-Zone quasi-dimensional model where sprays are divided on zones using both geometrical fundamentals, and mixture formation & evaporation conditions.**




RK-Model

# DIESEL – RK : combustion model possibilities

Advanced features of diesel combustion model:

1. Original multi-zone fuel spray combustion model (RK-model) which accounts:
   a - fuel properties including **bio-fuels** and blends of bio-fuels with diesel oil;
   b - few fuel injection systems in one cycle of **dual fuel** engine;
   c - detailed **piston bowl** shape;
   d - **swirl profile** and swirl intensity;
   e - injection profile, including **multiple injection** and PCCI / HCCI;
   f - number, **different diameters and directions** of nozzles holes;
   g - detailed **interaction of sprays** among themselves in volume and on walls accounting local walls temperatures.

2. **Detail Chemistry** simulation at **NOx** and Ignition Delay prediction.
3. Model of **Soot formation**.
4. Simulation of **Dual Fuel**; Gas; HCCI, **Assisted HCCI** engine concepts.

# DIESEL - RK

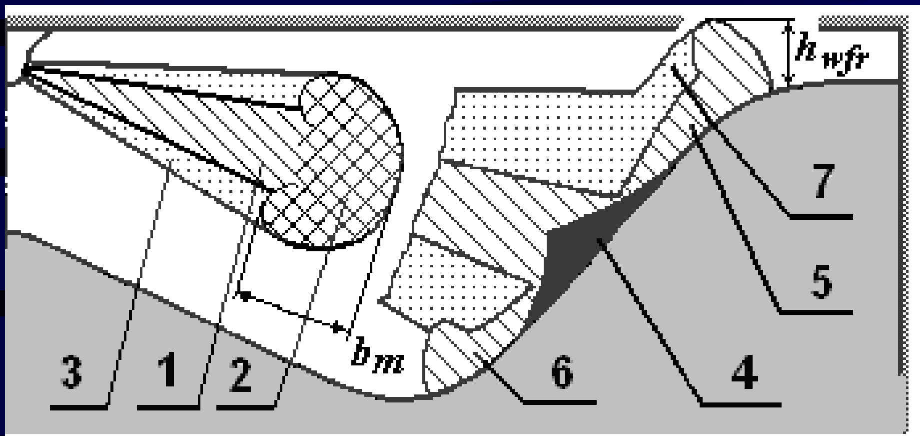
Options of ICE simulation tool:

- "Fuel Spray Visualization" code (animation of the simulation results).
- Built-in procedures of Multiparameteric optimization (15 methods of the nonlinear programming).
- Tool for express data file creation for different kinds of engines.
- Simulation of different combustion concepts:
  - Dual Fuel;
  - Gas;
  - PCCIO / HCCI;
  - Prechamber:
  - Assisted HCCI.

$l_{wj} = K_j B_{iw}^{0.5} \tau_w^{0.5}$

# Original multi-zone fuel spray model (RK-Model)

## Schematic Fuel spray structure




Publications:
- SAE 2005-01-2119;
- SAE 2006-01-1385;
- SAE 2007-01-1908;
- SAE 2009-01-1956;
- SAE 2013-01-0882;
- JSAE 20159169;
- JSAE 20159328.

## Character zones

Before spray and wall impingement:

1. Dense axial core of free spray.
2. Dense forward front.
3. Dilute outer sleeve of free spray.

After spray and wall impingement:

4. Axial conical core of NWF.
5. Dense core of NWF.
6. Dense forward front of NWF.
7. Dilute outer surroundings of NWF.

Additional zones

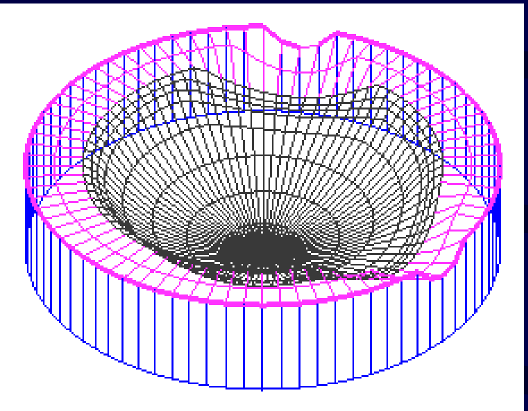
8. Fuel allocated on cylinder Head surface.
9. Fuel allocated on cylinder Liner surface.
10. Fuel allocated in crossing of NWF cores formed by adjacent sprays.
11. Fuel allocated in crossings of Fronts and Cores of free sprays.

* NWF is the so-called Near-Wall Flow of air with high density of fuel drops

# Representation of spray zones and piston bowl geometry

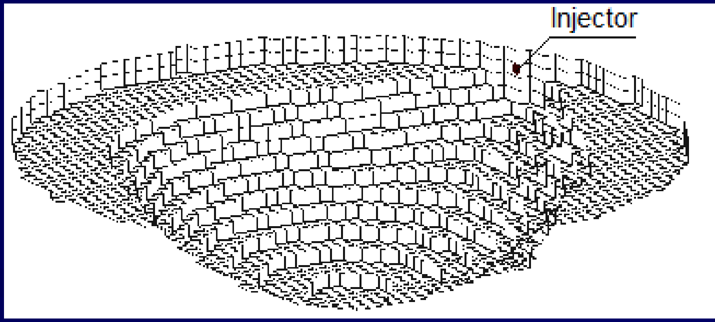
1. Analytical: - Piston bowl is set of straight cones and straight truncate cones.
- Spray zones are sets of sloping cones and loping truncate cones.

2. As a 3D mesh of cubic cells. Number of cells: ~ 80 per Cylinder Diameter

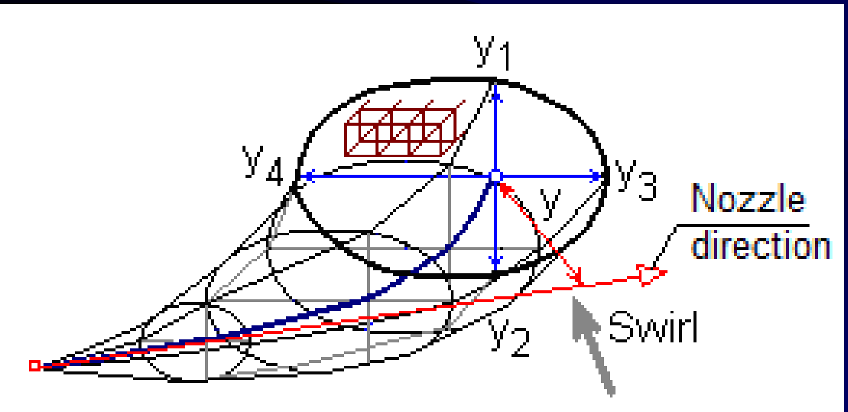


Piston crown with grooves for injectors in OP diesel 88-Г

… corresponding 3D mesh with cubic cells



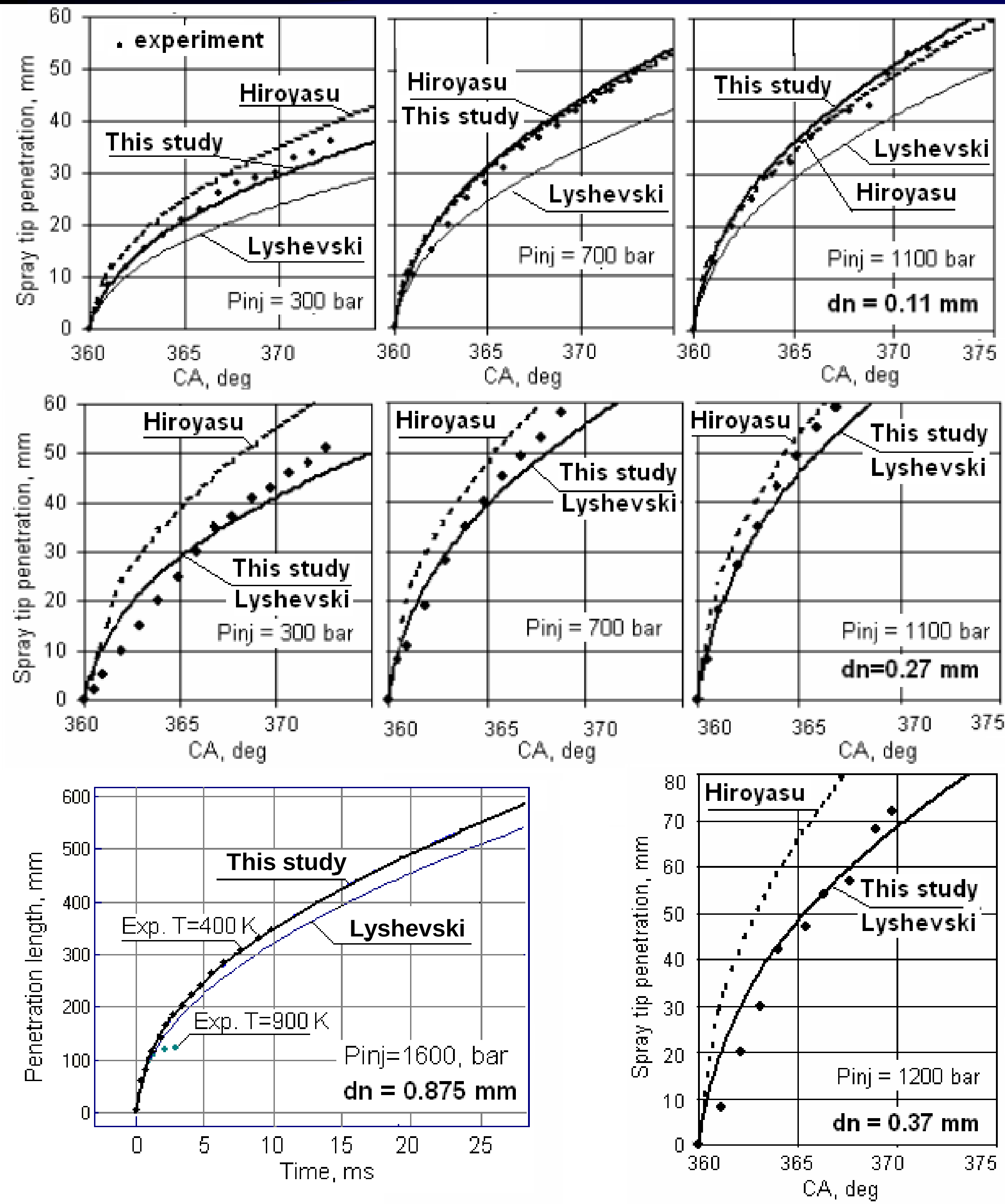

Spray is a set of cone and truncate cones




A volume of every spray zone is a sum of Volumes of all cells included into the zone.

The cells included into zones of few sprays simultaneously form zone of sprays intersection.

# Spray tip penetration modeling




Modified Lyshevski's equations using dimensionless parameters

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

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

$$Э = \tau_s^2 \sigma_f / (\rho_f d_n^3); \quad \rho = \rho_{air} / \rho_f ;$$

Penetration at break up: $l_a = A_s Э^{0.35} \exp[-0.2(\tau_s/\tau_g)];$

Penetration at main phase: $l_b = B_s^{0.5} \tau_s^{0.5};$

where: $A_s = 1.22 l_g Э_g^{-0.35}$

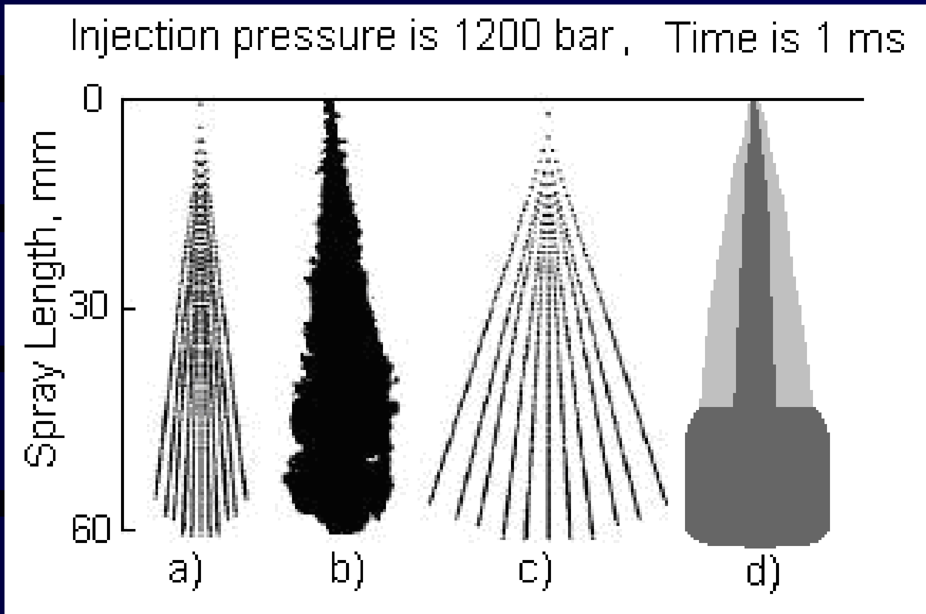
$$B_s = d_n U_{0m} We^{0.21} M^{0.16} / (D_s \sqrt{2} \rho);$$

$$D_s = \frac{14.21}{D_f \left[ \frac{-1.3511}{\exp(d_n)} + 0.68764 \exp(d_n) - 0.88869 \ln(d_n) \right]}$$

$d_n$ – nozzle bore, mm.

Experimental data:
SAE Pap. N 1999-01-0200.
SAE Pap. N 2000-01-0287.
SAE Pap. N 2002-01-0946
ILASS – Europe 2011, Estoril, Portugal, Sept. 2011.

# Free spray contour angle modeling




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) this study.

## Lyshevski's equations

$$\gamma_a = 2Arctg\left(E_s We^{0.35} M^{-0.07} \text{Э}^{-0.12} \rho^{0.5} e^{0.07\tau_s/\tau_g}\right);$$
$$\gamma_b = 2Arctg\left(F_s We^{0.32} M^{-0.07} \text{Э}^{-0.12} \rho^{0.5}\right)$$

Penetration at break up: $\gamma_a$

Penetration at main phase: $\gamma_b$

where: $E_s = 0.932 F_s We^{-0.03} \text{Э}_g^{0.12}$

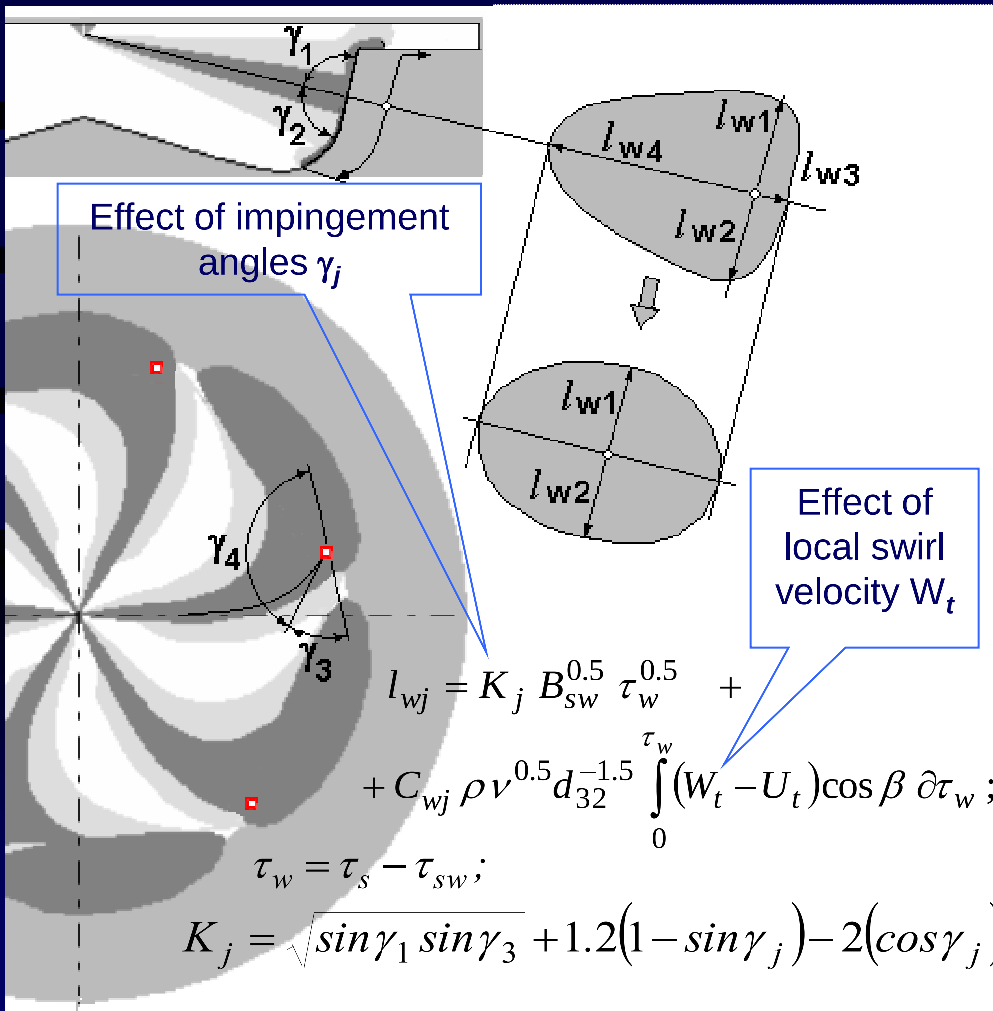
$Fs$ = 0.0075÷0.009

Usage of dimensionless parameters allows account properties of alternative fuels in simulation.


33. Reitz, R. D. and Bracco, F. B. On the Dependence of Spray Angle and Other Spray Parameters on Nozzle Design and Operating Conditions // SAE Paper 790494, 1979.
34. Dan T. The Turbulent Mechanism and Structure of Diesel Spray. Ph. D. Thesis, Toshisya University, 1996.
35. Dohoy Jung and Dennis N. Assanis. Multi-zone DI Diesel Spray Combustion Model for Cycle Simulation Studies of Engine Performance and Emissions // SAE Paper No 2001-01-1246, 2001.
36. Hiroyasu, H., and Arai, M. Fuel Spray Penetration and Spray Angle of Diesel Engines // Trans. of JSAE, Vol. 21, 1980, pp. 5-11.

# Simulation of the fuel sprays in the swirling air flow

Phenomenological Model of Interaction of Spray and their Near Wall Flow with Swirl and Walls.




$$l_{wj} = K_j \, B_{sw}^{0.5} \, \tau_w^{0.5} + C_{wj} \, \rho \, \nu^{0.5} d_{32}^{-1.5} \int_0^{\tau_w} (W_t - U_t) \cos\beta \, \partial\tau_w \, ;$$

$$\tau_w = \tau_s - \tau_{sw} \, ;$$

$$K_j = \sqrt{\sin\gamma_1 \, \sin\gamma_3} + 1.2(1 - \sin\gamma_j) - 2(\cos\gamma_j)$$

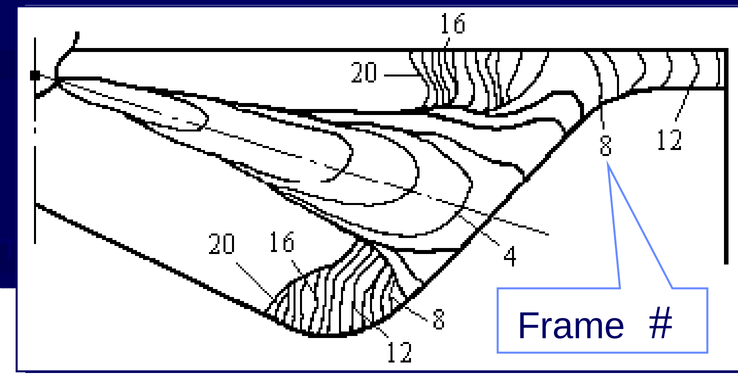
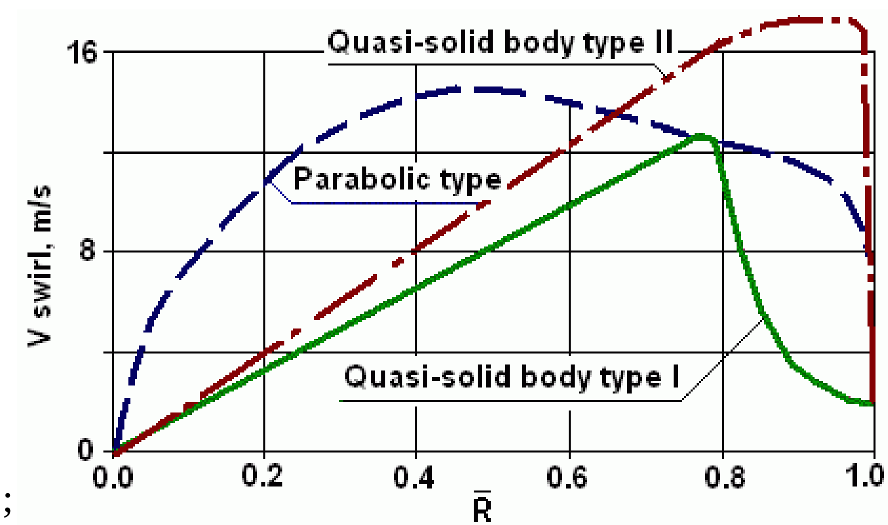


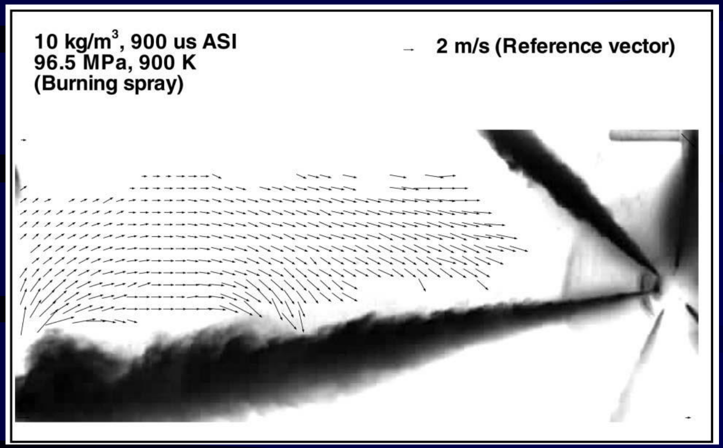

Photo-record obtained by V.V.Gavrilov

Swirl profiles

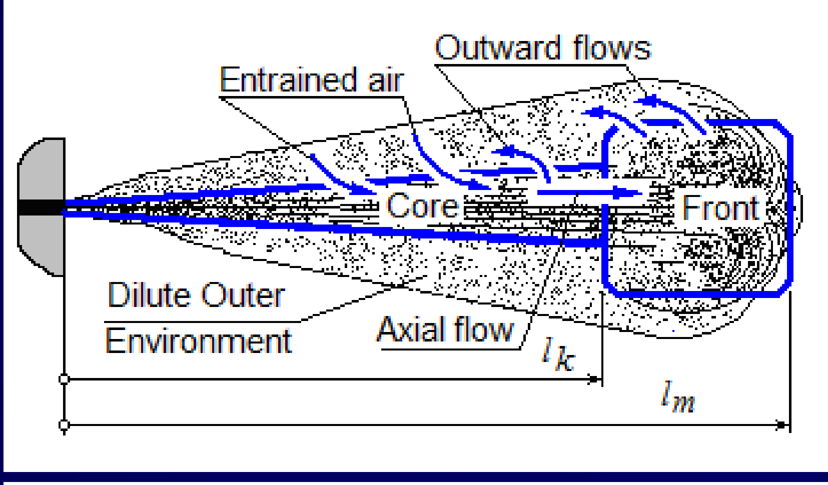



# Allocation of air in the character zones

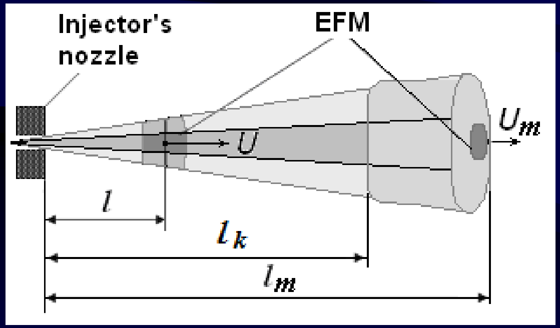
Air motion around fuel spray



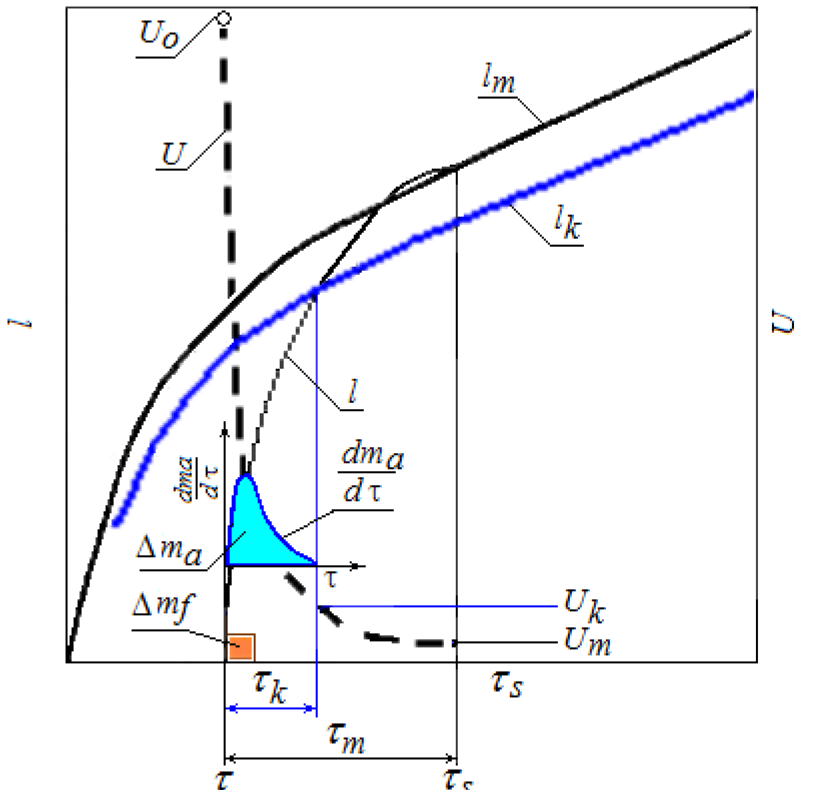

Scheme of air flows in a diesel spray




Motion of Elementary Fuel Mass (EFM) from injector to spray front zone $l_k$ and spray tip $l_m$.




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

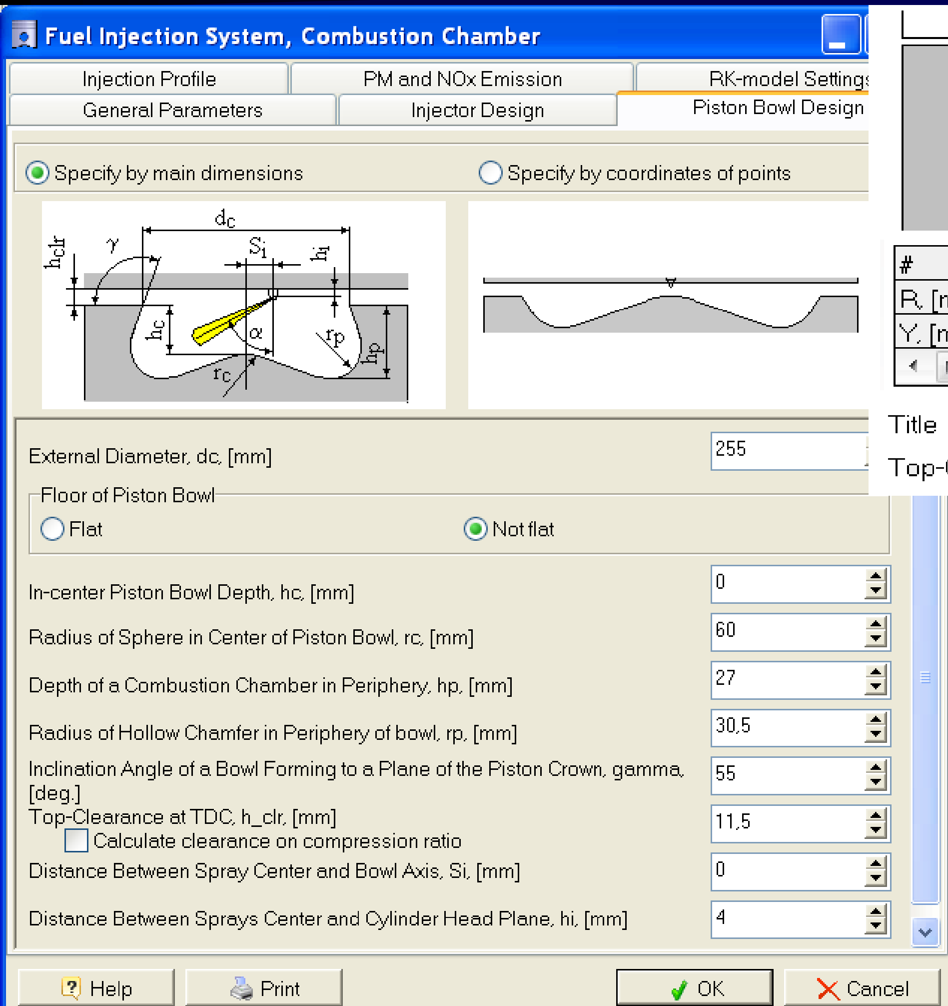



Mass of entrained air $\Delta m_a$ for every EFM $\Delta m_f$ is defined from momentum conservation:

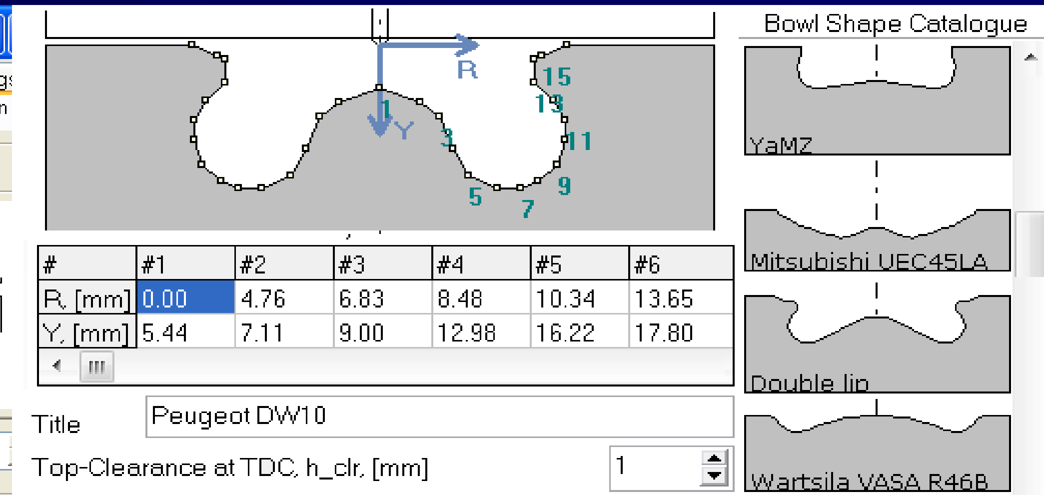
$$U_0 \, \Delta m_f = U_k \left( C_l \, \Delta m_f + \Delta m_a \right)$$

# Preprocessor for Piston Bowl Design Specification

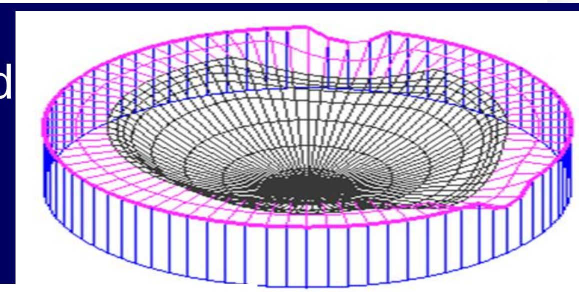
Specification by main dimensions

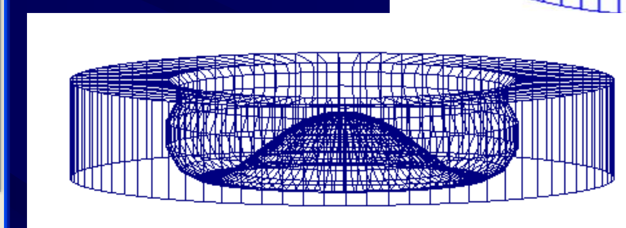



Specification by coordinates of points




3D mesh is used for piston bowl specification





Detailed geometry of piston bowl and configuration of nozzles holes allows definition of Coordinates and Time of spray with wall impingement.

# Allocation of fuel in the character zones

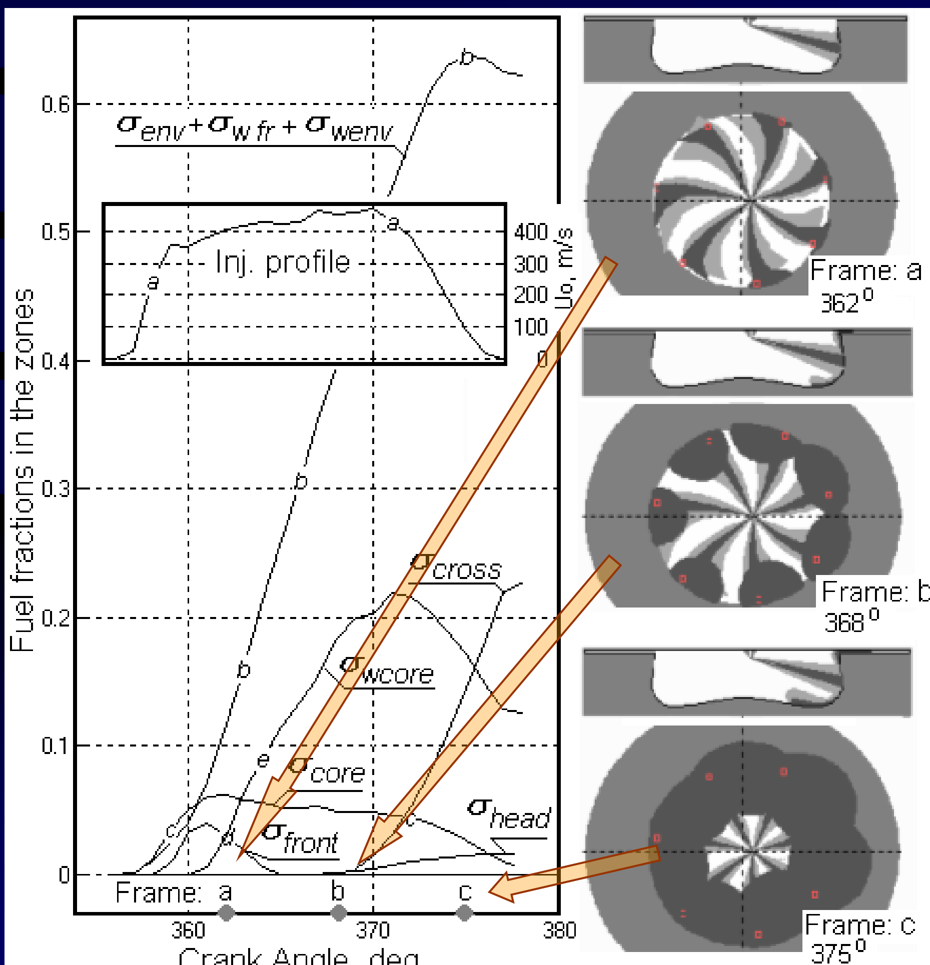
Truck diesel Yamz:

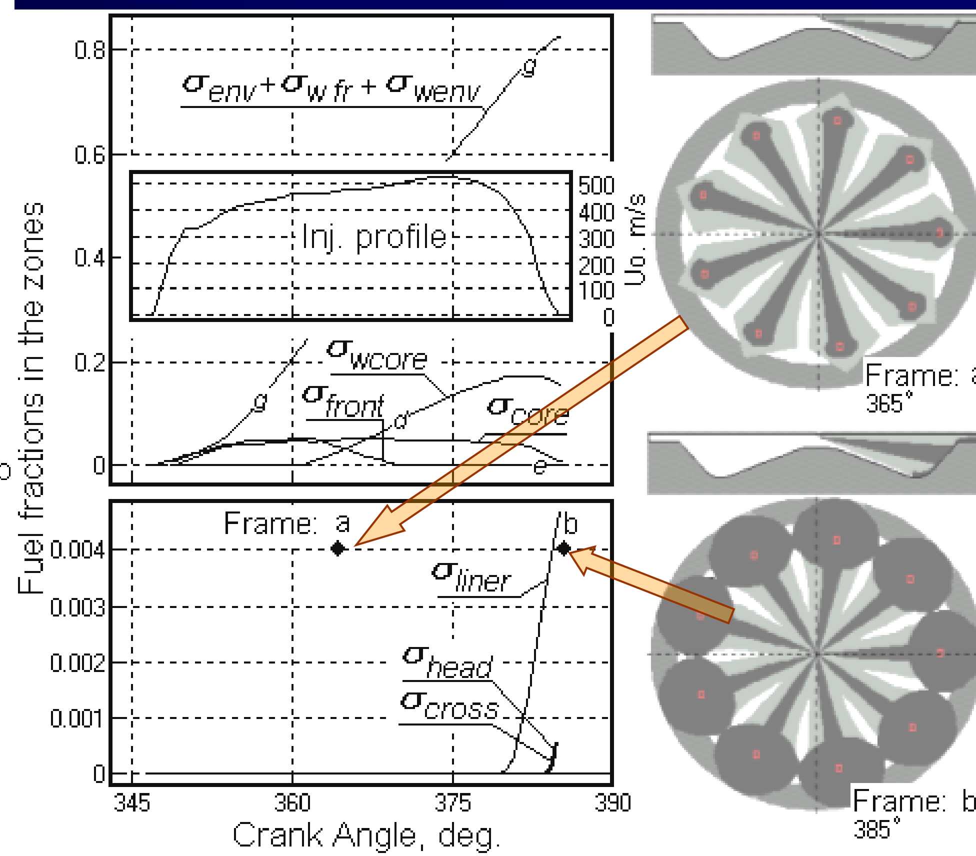
S/D=140/130, RPM=1700

Locomotive diesel Д49

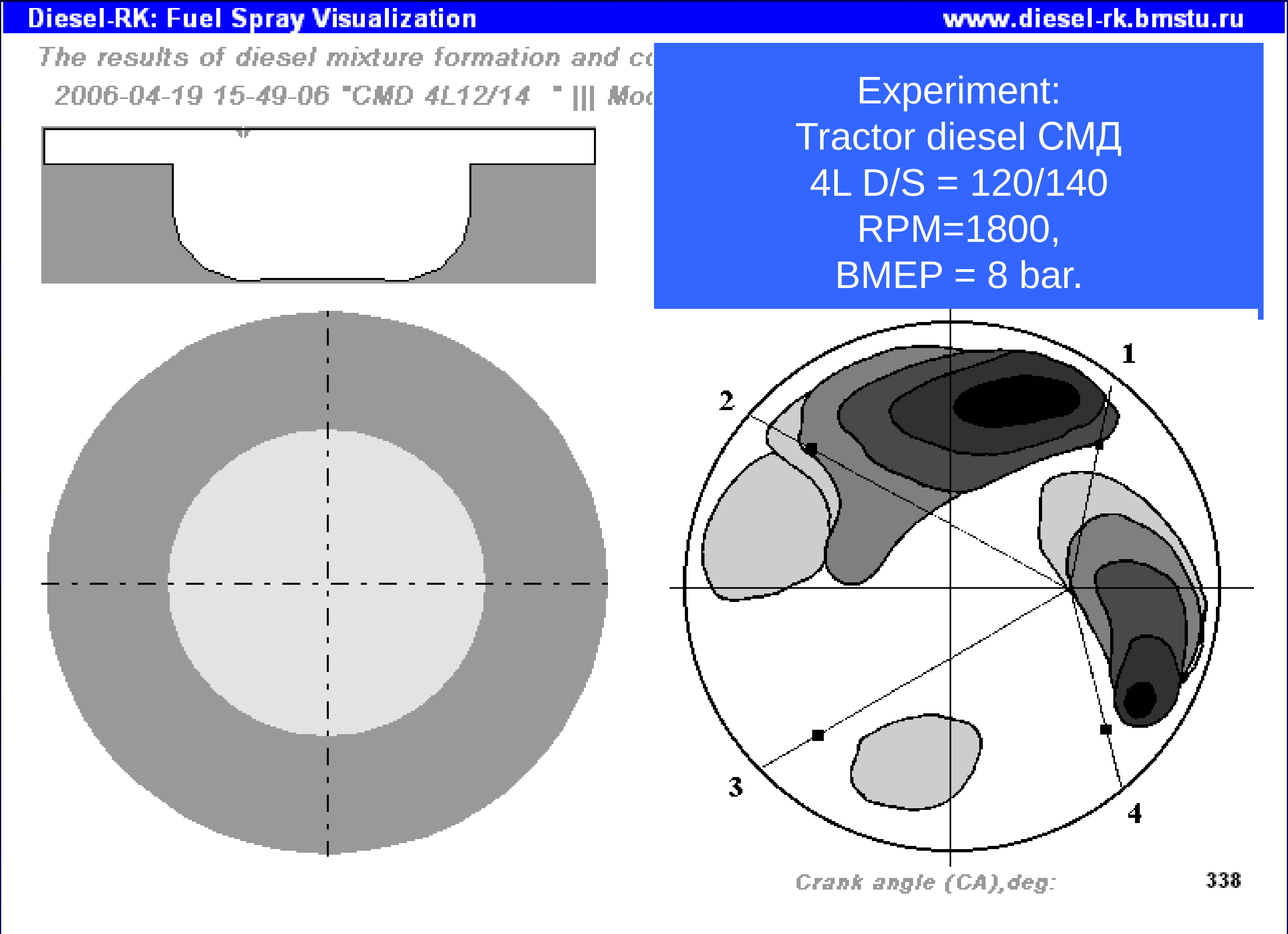
S/D = 260/260,

*RPM*=1000, BMEP=15 bar



# Visualization of sprays evolution with account the swirl

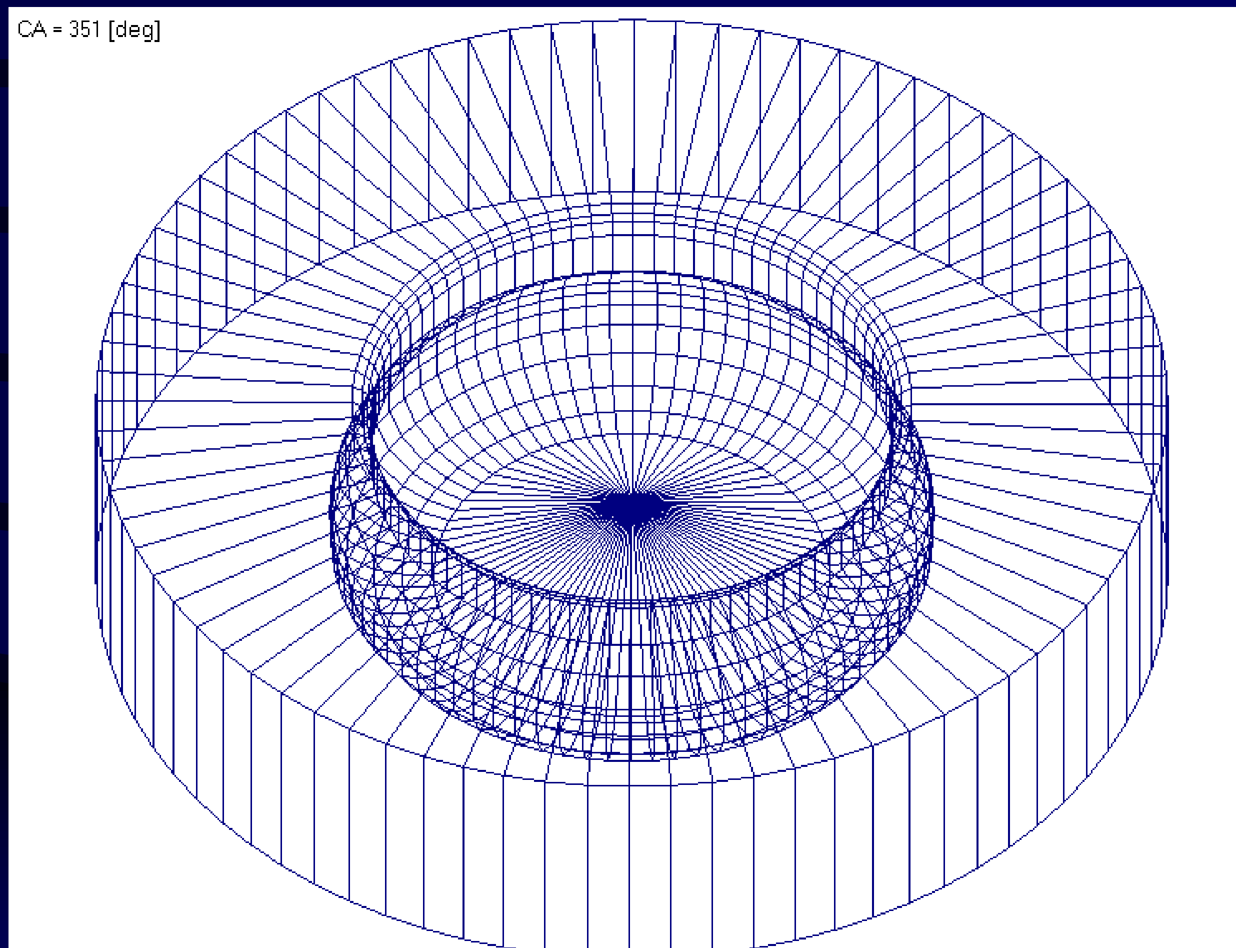



Experiment:
Tractor diesel СМД
4L D/S = 120/140
RPM=1800,
BMEP = 8 bar.

$l_{wj} = K_j B_{kw}^{0.5} \tau_w^{0.5}$

# 3D Fuel Spray Visualization code

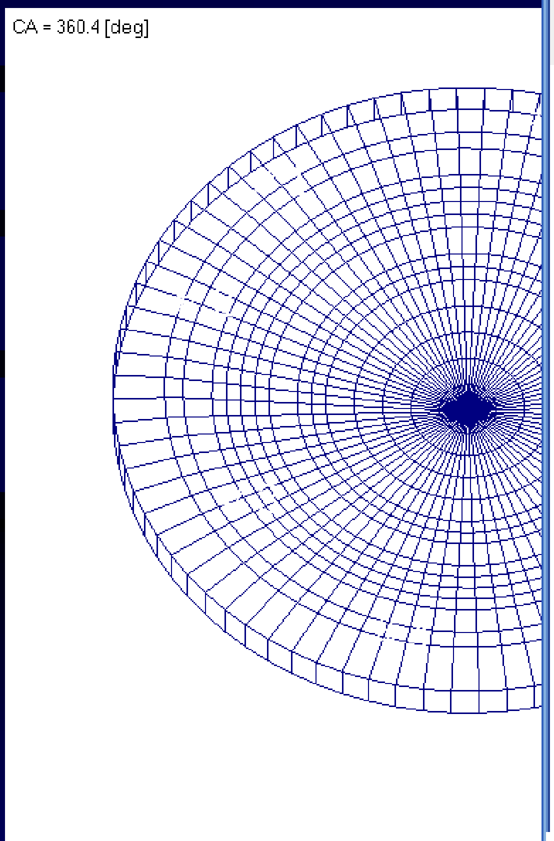
3D visualization allows rotate animation, zoom and highlight sprays and zones

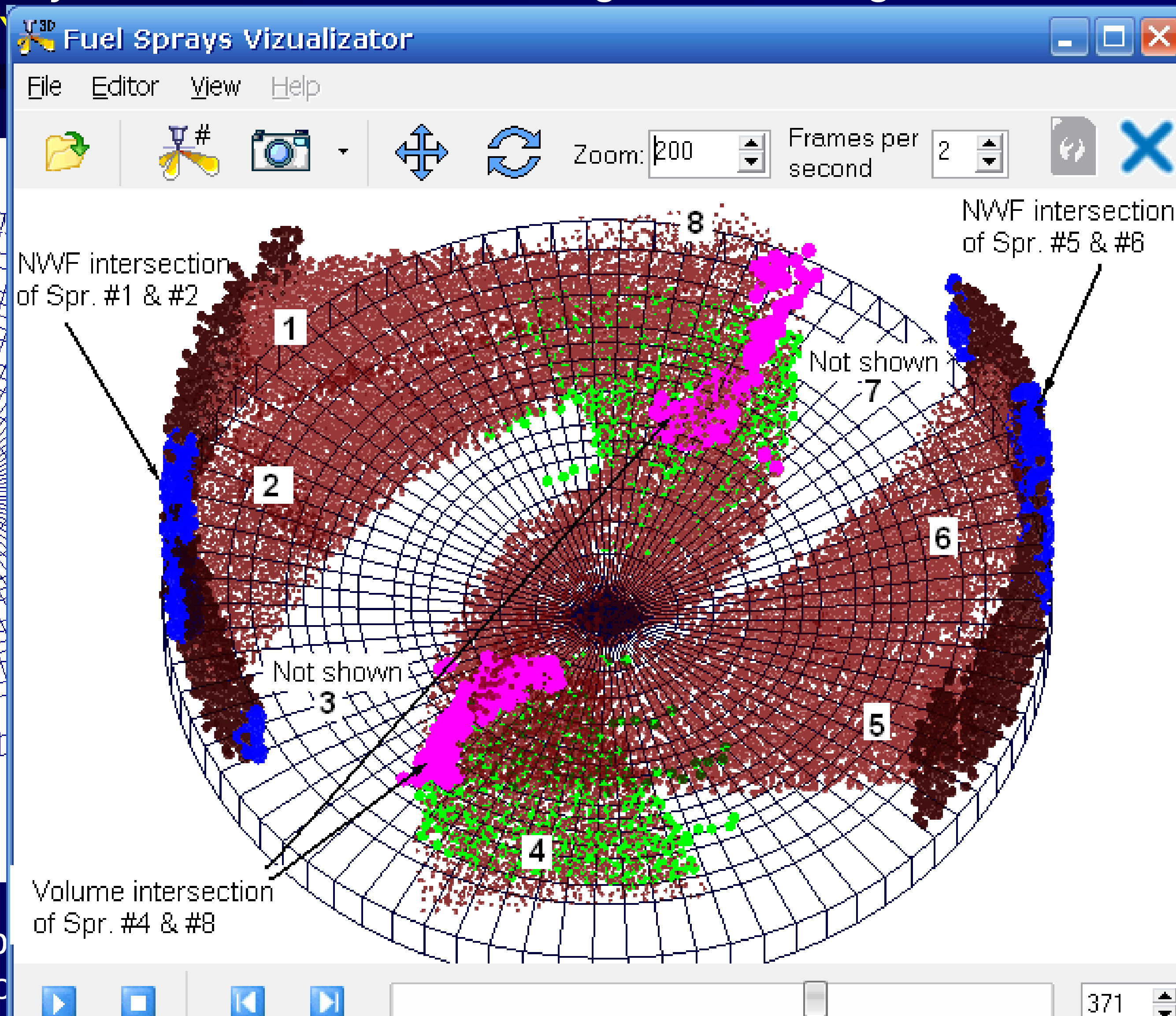



Computational time of spatial 7 sprays evolution simulation (in thermodynamic cylinder model) is about 1 minute !

# Fuel Spray Visualization code

3D visualization of sprays evolution in 2 stroke large marine engine with 2 injectors in cylinder.



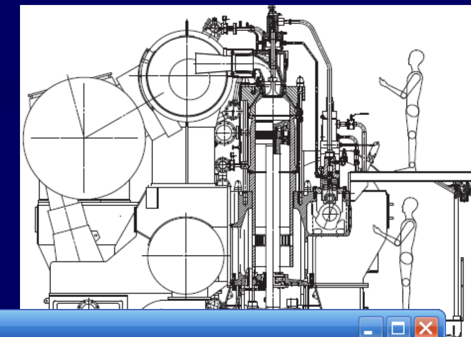



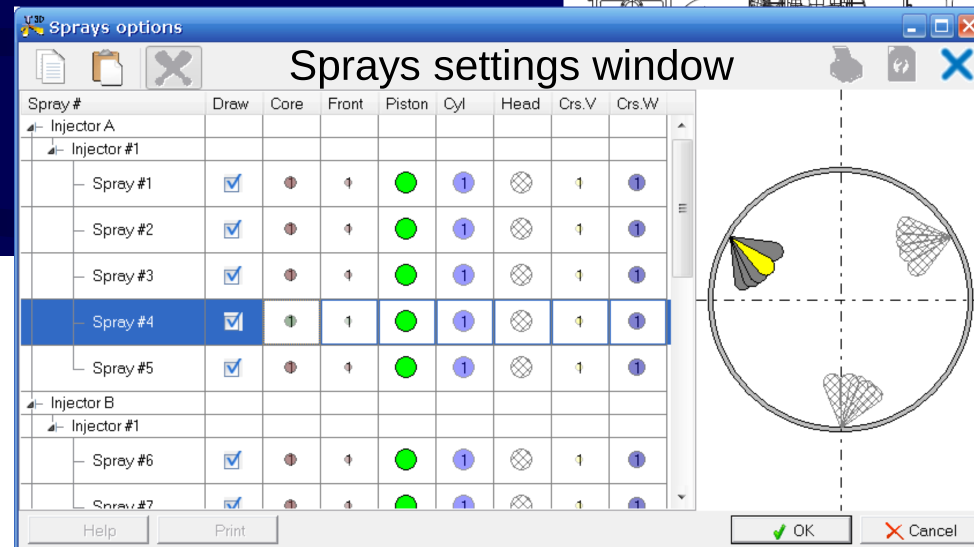

Dark Green bullets mark sp
Dark Blue – their intersectio

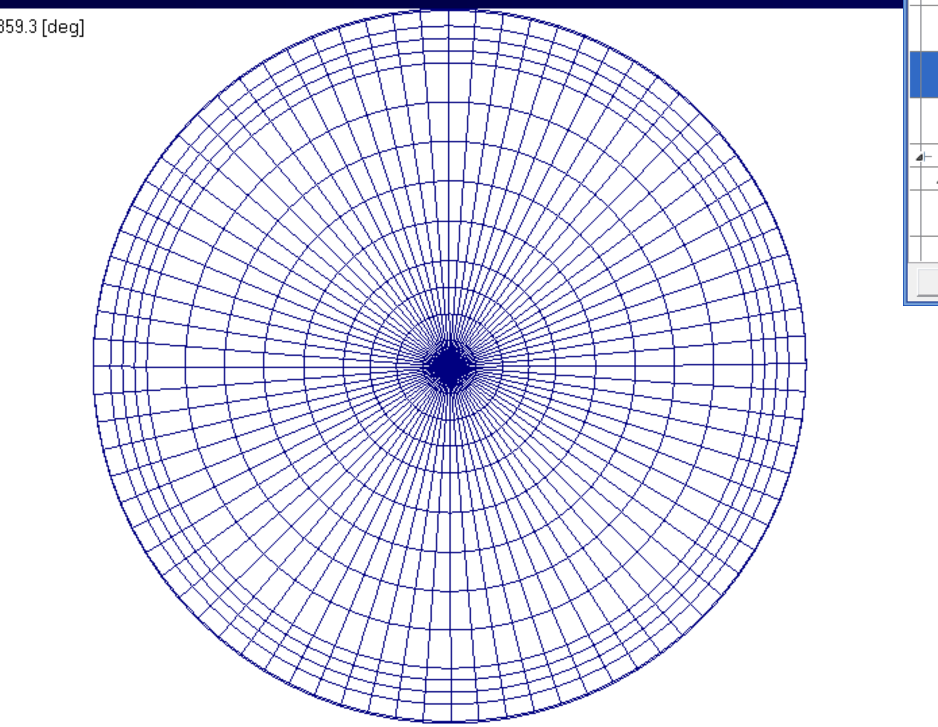
# 3D Fuel Spray Evolution

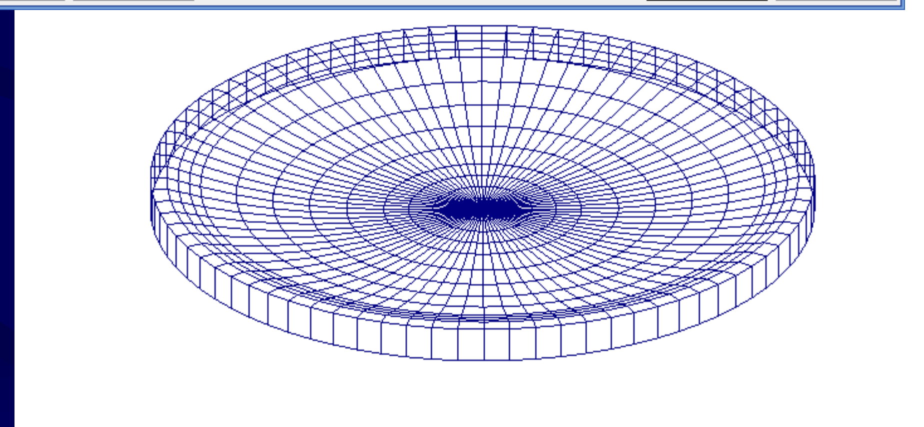
3D visualization of sprays evolution in 2 stroke large marine engine with 3 injectors in cylinder.

Yellow bullets mark spatial intersection of sprays





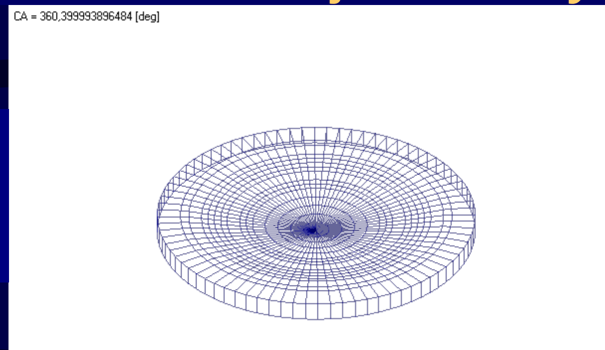



Dark Green bullets mark spray # 4, #9 & # 14; Blue bullets mark Near Wall Flows on cylinder head; Dark Blue – their intersections

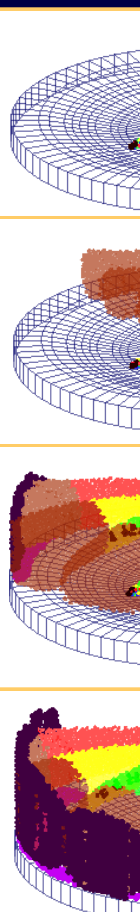
# Effect of Spatial intersection of sprays on HRR in engine with side injection system

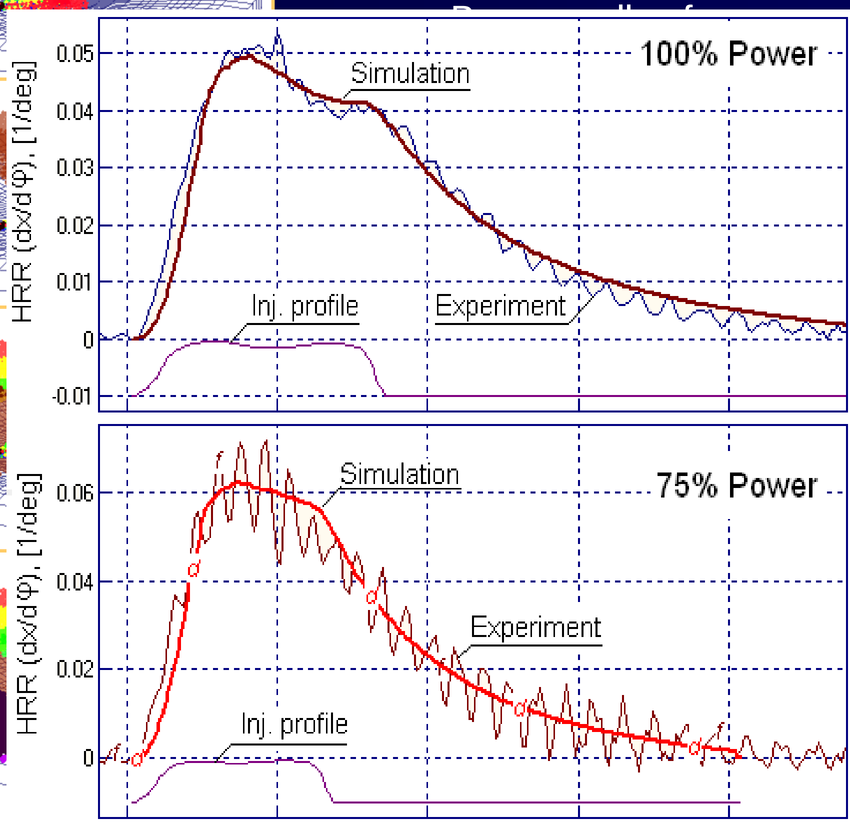
Red, Yellow, Green and Blue are cells of sprays core.

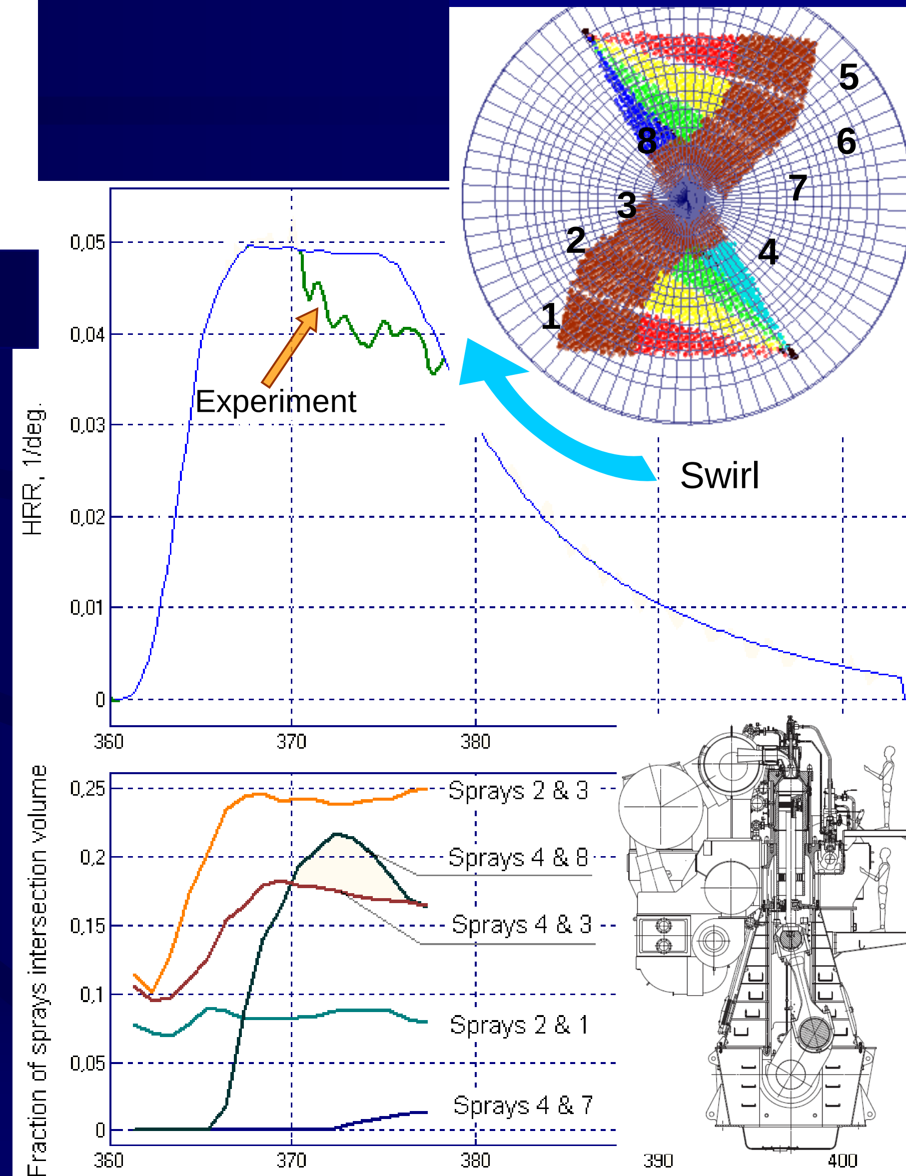



$361^0$

View from bottom (through piston)

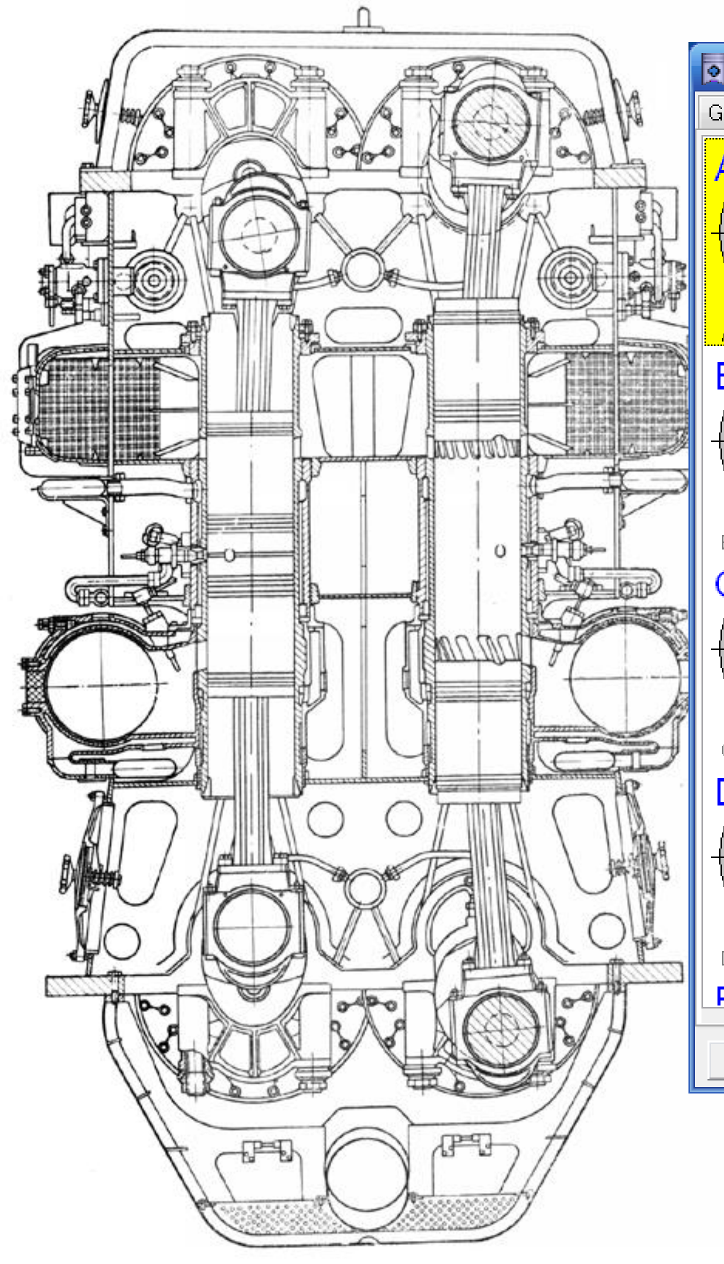


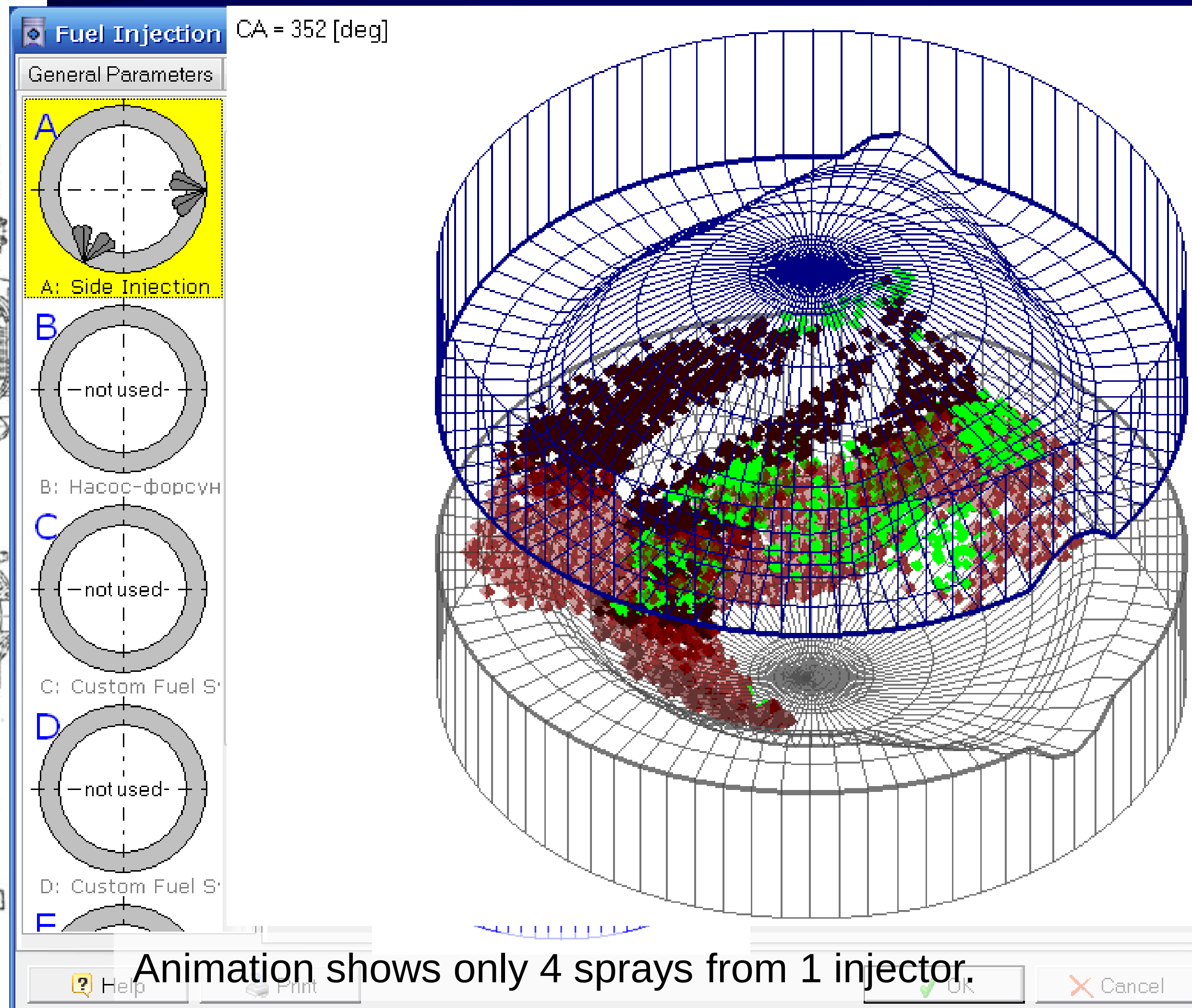


# Simulation of combustion in OP engine

18 L D/S = 230 / 2x300       6700 kW @ 900 RPM

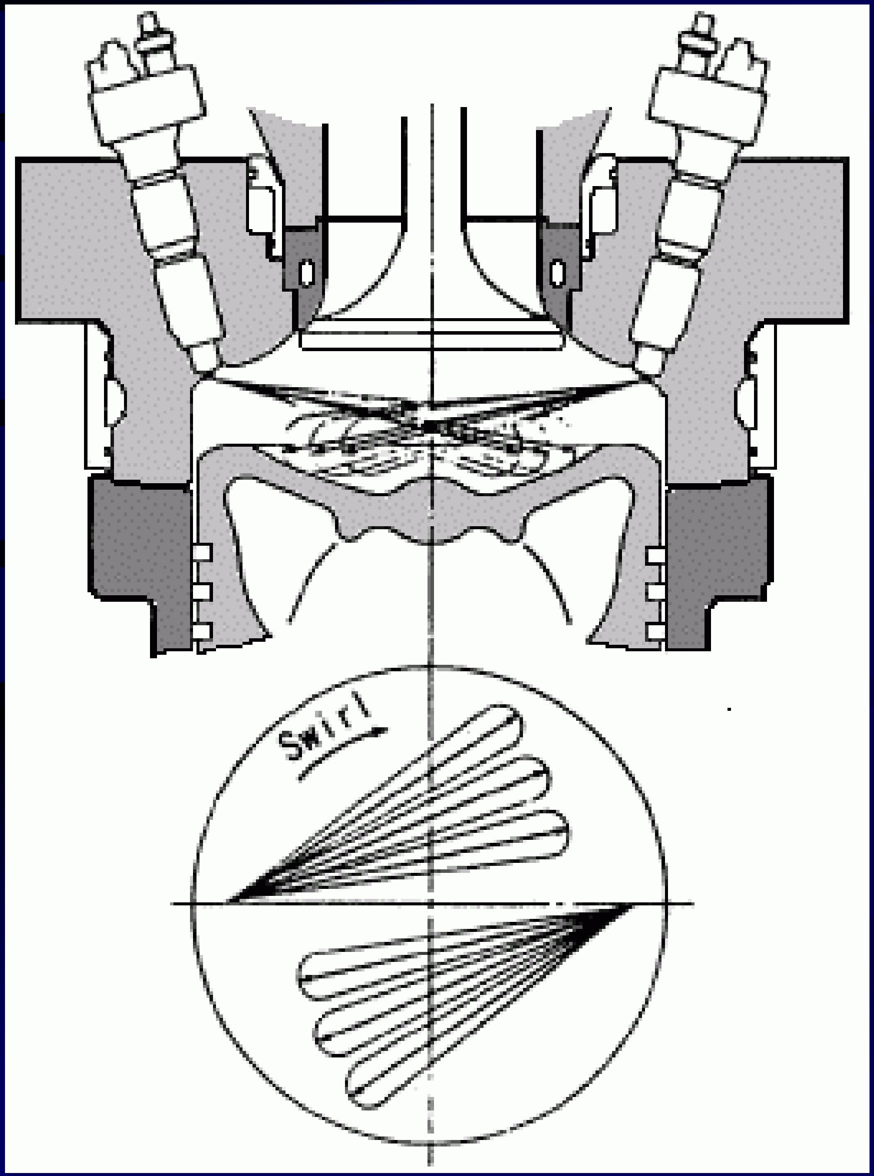




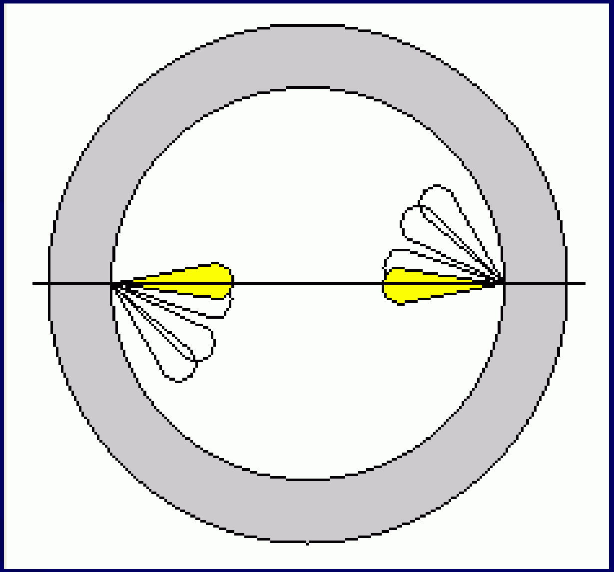

Animation shows only 4 sprays from 1 injector.

- Green bullets show intersection of the sprays

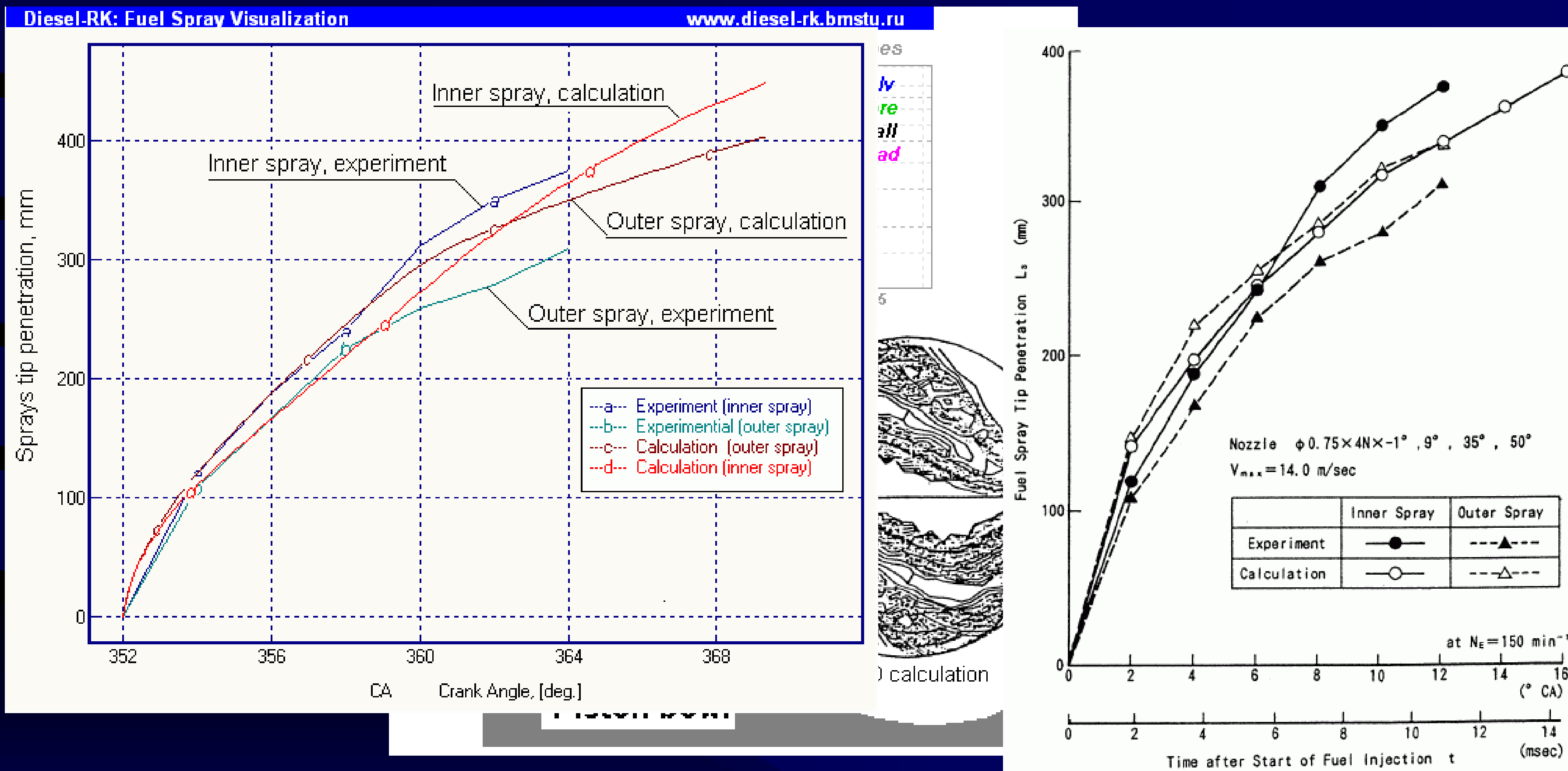
# Simulation of fuel spray motion and combustion in two-stroke diesel with side injection system




Engine: Mitsubishi UEC 45 LA
D = 450 mm    S = 1350 mm
RPM = 158;
2 injectors: 4 x 0.75
Angles of holes in above view:
$50^0$ , $35^0$, $9^0$, $-1^0$



# Results of simulation of fuel sprays evolution with DIESEL-RK software in comparison with published CFD simulation and experiment

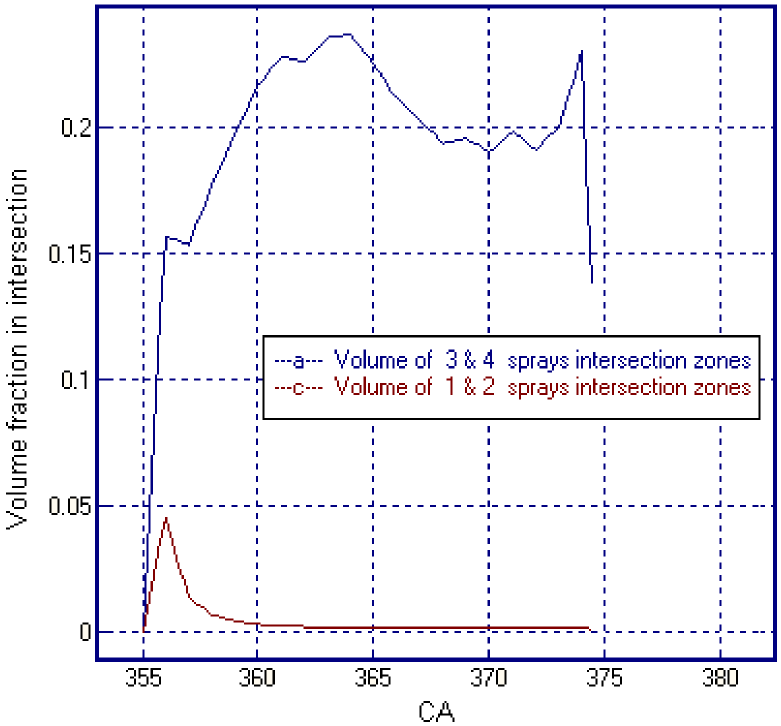


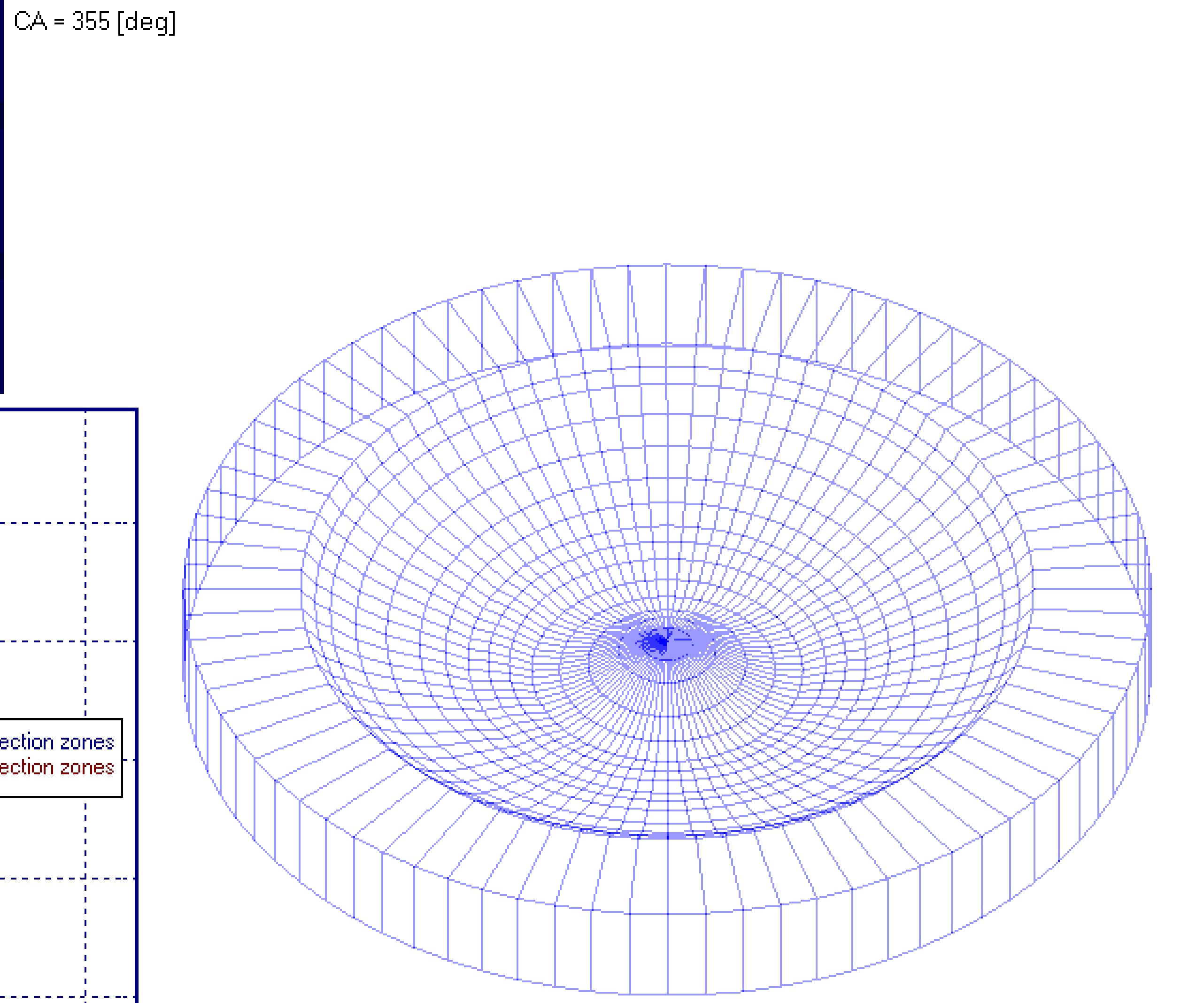

**H.Nakagawa, Y.Oda, S.Kato, M.Nakashima and M.Tateishi: "Fuel Spray Motion in Side Injection Combustion System for Diesel Engines", International Symposium COMODIA 90, pp. 281-286, 1990.**

# 3D Fuel spray visualization

Mitsubishi UEC 45 LA
D = 450 mm  S = 1350 mm
RPM = 158;
2 injectors: 4 x 0.75
Angles of holes in top view:
$50^0$ , $35^0$, $9^0$, $-1^0$

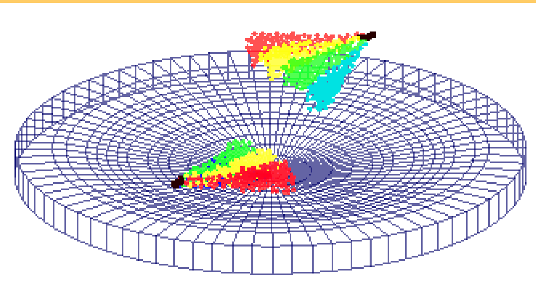
Intersections of sprays:
(**Yellow markers**).



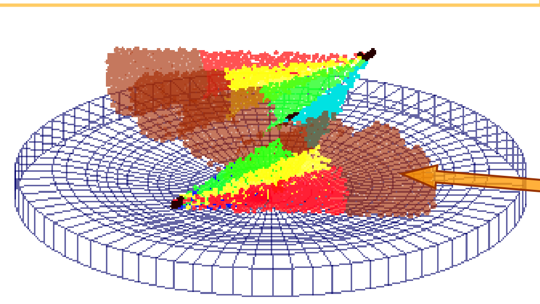



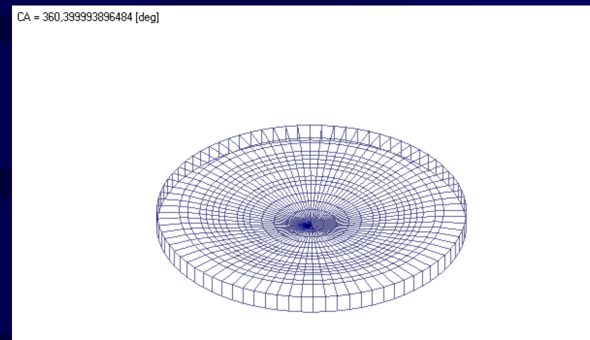
# 3D visualization of sprays evolution in diesel with side injection system

Red, Yellow, Green & Blue bullets are sprays core zones cells.



$361^0$

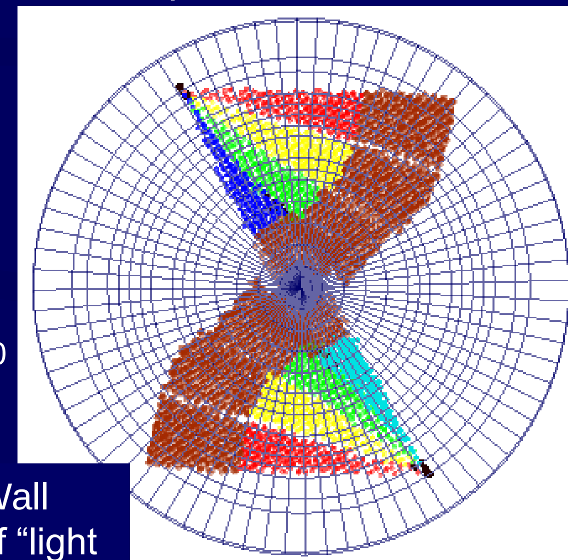




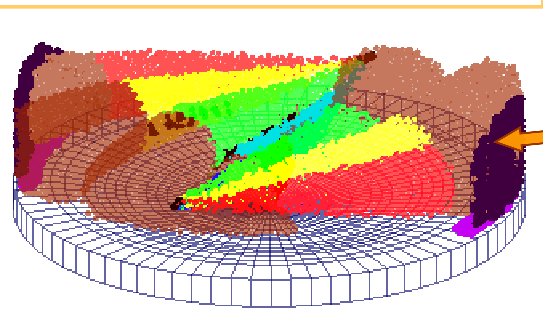

$363^0$

Brown bullets are Sprays Front Zones Cells.

Bottom view through piston surface



$363^0$

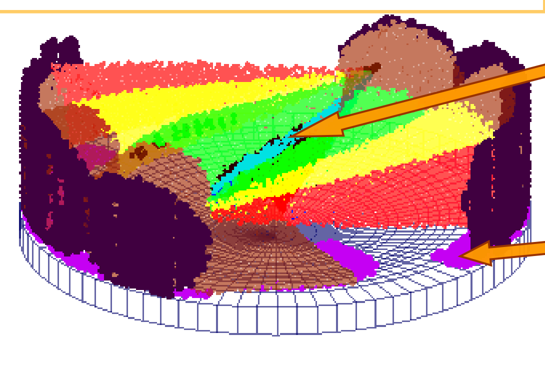


$367^0$

Zones of Near Wall Flow on the Cylinder Liner.

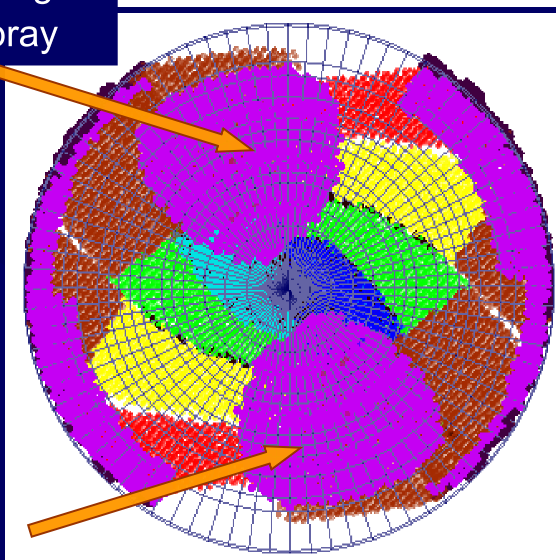
Near Wall Flow of “light blue” spray

Black bullets are the cells where the spray cores intersect each other.



$371^0$

Prune Bullets are Zones of Near Wall Flow on the piston surface



$371^0$

Near Wall Flow of “blue” spray

# Calculation of the zone temperature

Energy balance equation for every zone of the spray:

$$\Delta U_a + \Delta U_{lf} + \Delta U_{vf} = \Delta Q_{a\,IN} + \Delta Q_{lf\,IN} + \Delta Q_{vf\,IN} - \Delta Q_{a\,OUT} - \Delta Q_{lf\,OUT} - \Delta Q_{vf\,OUT} - $$
$$- p\Delta V - H_{evap} + \Delta Q_X$$

where: $\Delta U$ is difference of internal energy at the end and start of time step;
$\Delta Q_{IN}$ is energy, delivered into zone; $\Delta Q_{OUT}$ is energy, removed from zone;
$p$ is a pressure, $\Delta V$ is variation of the zone volume; $H_{evap}$ is a heat for droplet evaporation;
$\Delta Q_X = m_{vf\,2}\,\xi_b\,H_U$ is heat of combustion of fuel vapor in the zone.

$\Delta Q_X = m_{vf\,2}\,\xi_b\,H_U$

Indexes: $a$ – gas (air); $lf$ – liquid fuel; $vf$ – fuel vapor; $fe$ – evaporated fuel;
$1$ and $2$ mean start and end of time step; $IN$ and $OUT$ are delivering and removing.

The diameter of the fuel droplets after evaporation during time step $d\tau$:

$$d_{32\,2} = \sqrt{d_{32\,mix}^2 - K_i\,d\tau}$$

The diameter of the fuel droplets (SMD) in the zone after their mixing; here $N$ is a number of droplets in zone.

$$d_{32\,mix} = \frac{N_1 d_{32\,1}^3 + N_{IN} d_{32\,IN}^3}{N_1 d_{32\,1}^2 + N_{IN} d_{32\,IN}^2}$$

The mass of evaporated fuel is calculated using diameters of fuel droplets prior and after evaporation:

$$\Delta m_{fe} = \left(m_{lf\,1} + \Delta m_{lf\,IN}\right)\left[1 - \left(\frac{d_{32\,2}}{d_{32\,mix}}\right)^3\right]$$

# Modeling of evaporation

Evaporation rate of droplet is described by Sreznevski's equation:

$$d_{32\,2} = \sqrt{d^2_{32\,mix} - K_i\, d\tau}$$

where $d_{32}$ is a current Sauter Mean Diameter of droplets;
$d\tau$ is a time step.

$K_i$ is evaporation constant (every i-zone has own $K_i$)

$$K_i = 4\cdot 10^6\, Nu_{Di}\, D_{pi}\, p_{Si} / \rho_f$$

$Nu_D$ is Nuselt number for diffusion process (Sherwood number). Every zone has own $Nu_D$.

$D_p$ is Diffusion Coefficient (every zone has own $D_{pi}$) :

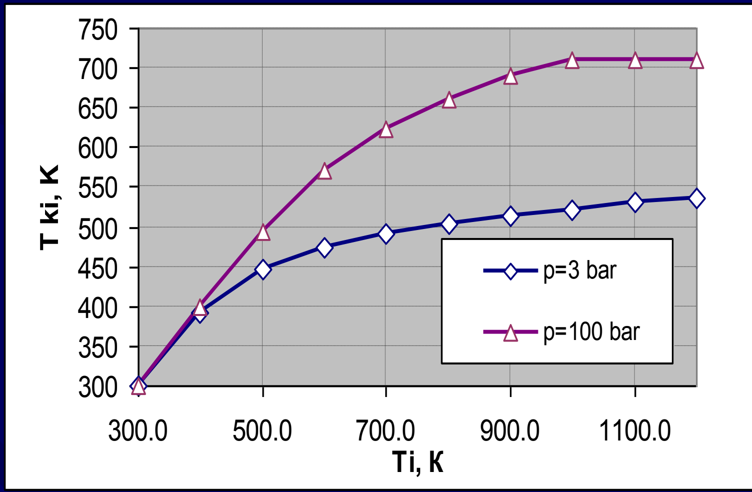
$$D_{pi} = D_{po}\left(T_{ki}/T_o\right)\left(p_o/p\right)$$

$D_{pi}$ depends on Equilibrium Evaporation Temperature $T_{ki}$ and current pressure $p$;

$p_{Si}$ is Saturated Vapor Pressure at the temperature $T_{ki}$ (every zone has own $p_{Si}$).

$T_{ki}$ of i - zone is calculating using energy balance around a droplet (express. of Virubov D.N.):

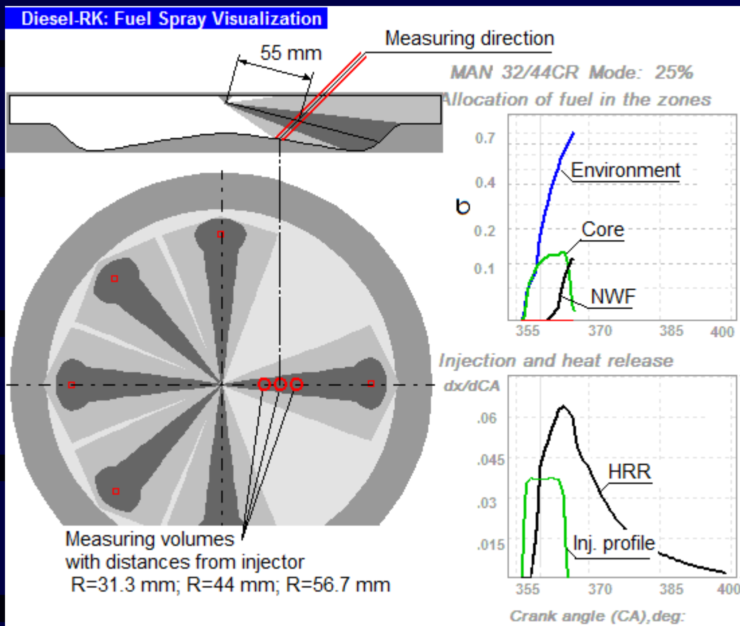
$$\lambda_a\left(T_i - T_{ki}\right) = D_{pi}\, p_{Si}\left[C_f\left(T_{ki} - T_f\right) + h_{evap} + C_{fv}\frac{T_i - T_{ki}}{2}\right]$$

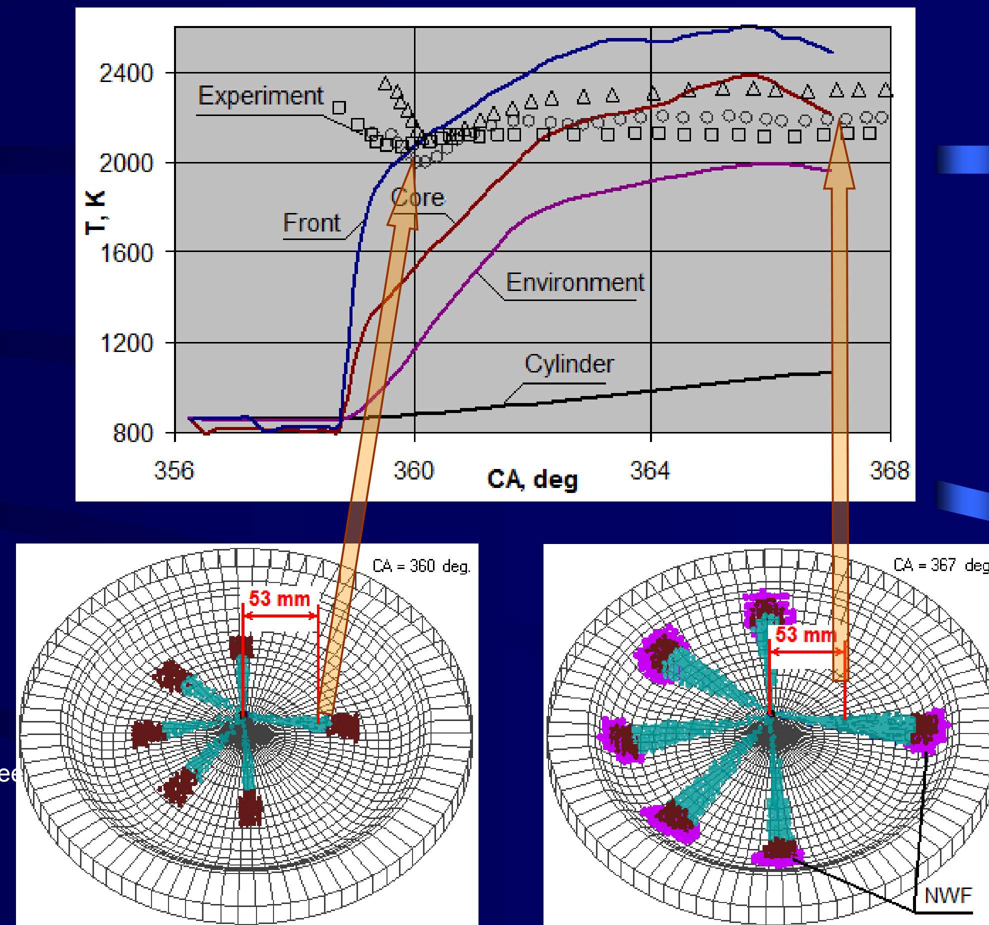



where: $\lambda$ is heat conductivity at $T_{ki}$ ; $T_i$ is character temperature of *i*-zone; $C_f$ and $C_{fv}$ are heat capacity of fuel and fuel vapor, $T_f$ is injected fuel temperature.

# Validation of results of numerical modeling

## 1 cyl MAN test engine D/S=320/440; RPM=750; BMEP=6.54 bar [*]




Сгорание начинается при CA ≈ 358.5 град. Однако, в расчете не получается столь резкого скачка температуры во фронте струи, как это фиксирует измерение, возможно в алгоритме расчета не достаточно оценена степень выгорания паров топлива $\xi_b$ в начальный момент объемного сгорания. Тем не менее, расчетная температура в зоне фронта струи близка к экспериментальному значению. Позднее, при CA > 360 град. относительно более горячий передний фронт струи уходит из зоны измерения вперед, и его место замещает более холодное ядро струи. (Задняя граница зоны фронта струи удаляется более чем на 55 мм от форсунки.) Фиксируемая температура в зоне измерения в это время остается высокой, она заметно превышает среднюю расчетную температуру ядра, по крайне мере до момента времени CA ≈ 362 град., рис. 13. Отличие температур в данном случае объясняется тем, что температура в ядре не равномерно распределена по его длине: чем ближе к фронту струи, тем выше температура. А именно головная часть ядра попадает в зону измерения до момента CA ≈ 362 град., что подтверждается и результатами визуализации развития струи. В расчетных же данных фигурирует средняя температура по объему зоны. Позднее, при CA > 362 град., когда в зону измерения попадает уже основной объем (срединная часть) ядра струи, расчетная средняя температура ядра струи практически совпадает с результатами измерений. В результате следует отметить, что расчет достаточно точно отражает температуру внутри струи, а значит и процессы массообмена, испарения и сгорания внутри струи.

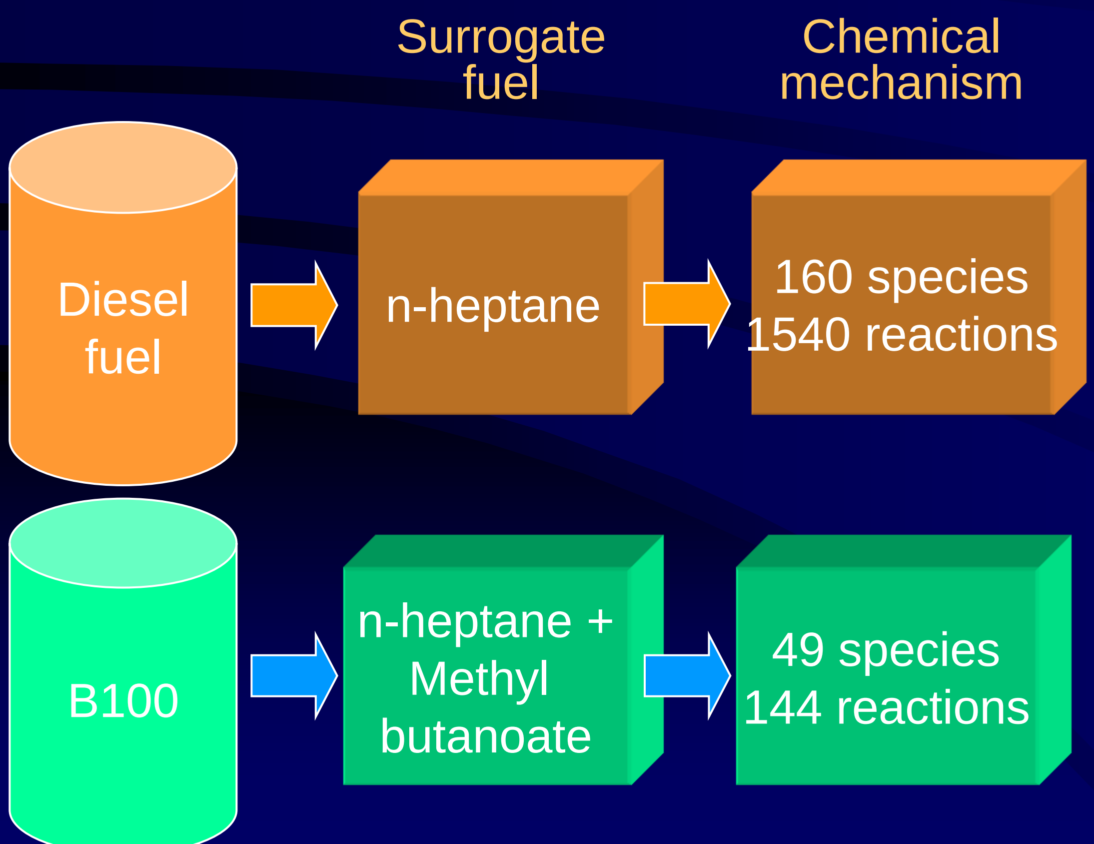
* Fridolin Unfug, Uwe Wagner, Kai W. Beck, Juergen Pfeil, Ulf Waldenmaier, Oguz Celik, Johannes Jaeschke and Juergen Metzger. Investigation of Fuel Spray Propagation, Combustion and Soot Formation/Oxidation in a Single Cylinder Medium Speed Diesel Engine // ASME 2012 Internal Combustion Engine Division Fall Technical Conference, Vancouver, BC, Canada, September 23–26, 2012.

# Improved ignition delay calculation

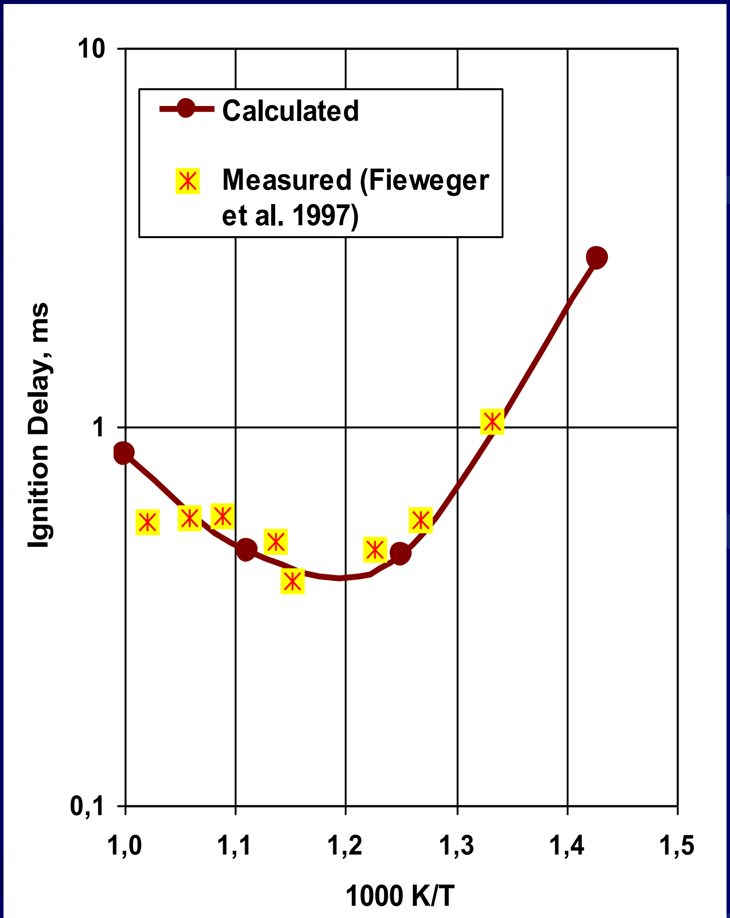
For engines with PCCI / HCCI the existing empirical equations for Ignition Delay prediction can not be used and Detailed Chemistry Model was developed and implemented.

The Lawrence Livermore National Laboratory (LLNL) mechanism is used for diesel fuel.
At every time step the delay is calculated taking into account:

- Pressure,
- Burnt Gas Fraction (EGR),
- Temperature,
- Air/Fuel Ratio.




Calculation for n-heptane (Diesel)



# Low temperature combustion simulation

Low Temperature Combustion (LTC) Model is used when High Temperature Combustion (HTC) ignition delay exceeds some value. For engines with PCCI / HCCI the LTC delay $\Theta_{iLTC}$ is function of HTC delay $\Theta_{iHTC}$ and EGR fraction $C$:

$$\Theta_{iLTC} = 8.281 + 1.0259\,\Theta_{iHTC} - 4.8822 \ln \Theta_{iHTC} - \sqrt{31.602\,C}$$

Fraction of fuel burning by LTC mechanism can be calculated with expression derived by processing published data:

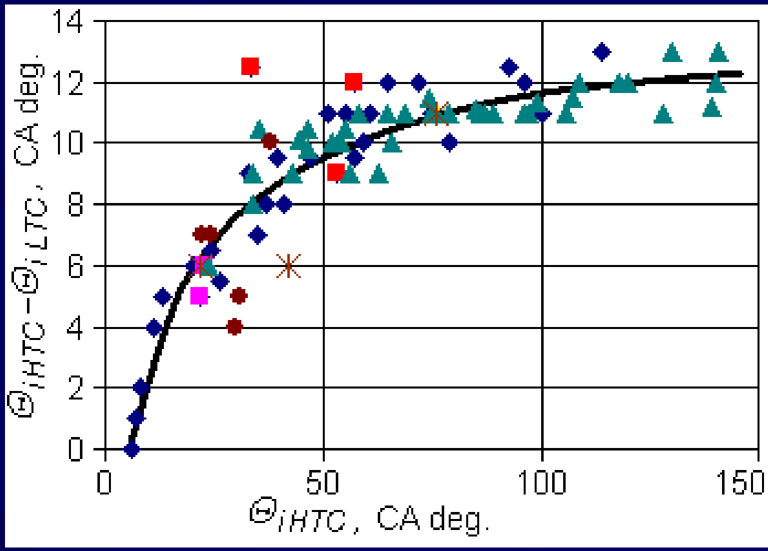
$$x_{LTC}^{\max} = (0.102 - 0.0392\,C) \cdot \left( \frac{81.6}{\exp \Theta} - \frac{8.88}{\Theta} + 1.2261 \right)$$

where $\Theta = MAX\,(6.7,\ \Theta_{iLTC})$.

Heat release of LTC can be approximated with Wiebe expression, as a function of crank angle $\varphi$ varied from the beginning of LTC (where $\varphi = 0$) up to $\varphi_z$.

$$x_{LTC}(\varphi) = x_{LTC}^{\max} \left\{ 1 - \exp\left[ -2.9957 \left( \frac{\varphi}{\varphi_z} \right)^{m_v + 1} \right] \right\}$$

where: $m_v = 1.2 + 0.69\,C$ is a mode of Wiebe function; $\varphi_z$ = 6…8 CA deg is a duration of the LTC.

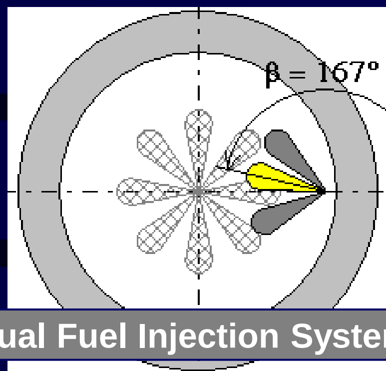



*Citation: Kuleshov A.S. Multi-Zone DI Diesel Spray Combustion Model for Thermodynamic Simulation of Engine with PCCI and High EGR Level // SAE Tech. Pap. Ser. – 2009. – N 2009-01-1956. – P. 1-21.*

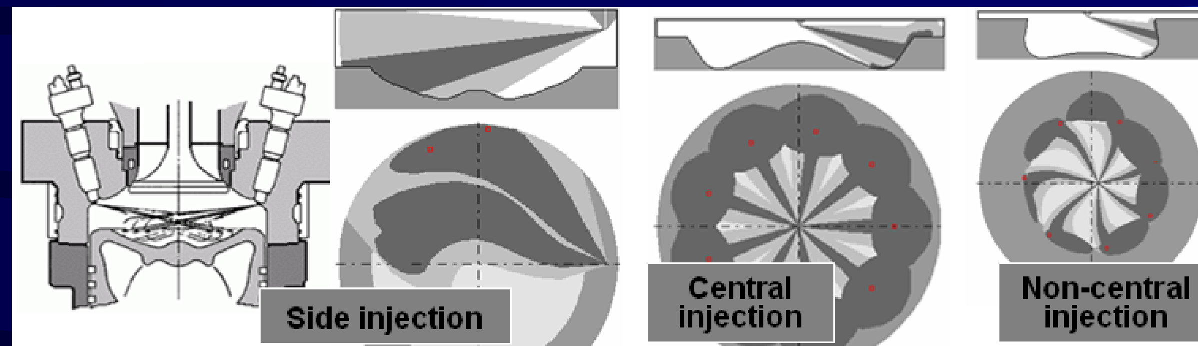
# Engine simulation software possibilities

Full cycle thermodynamic engine simulation tool DIESEL-RK has following features for combustion optimization:

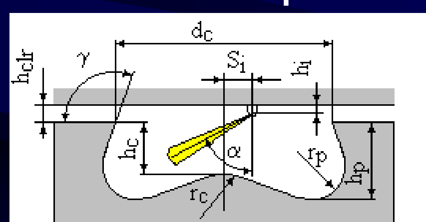
- Any location of sprayers.



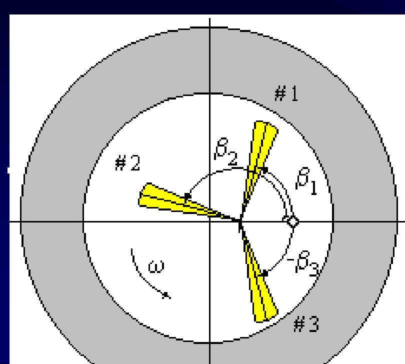

Dual Fuel Injection System

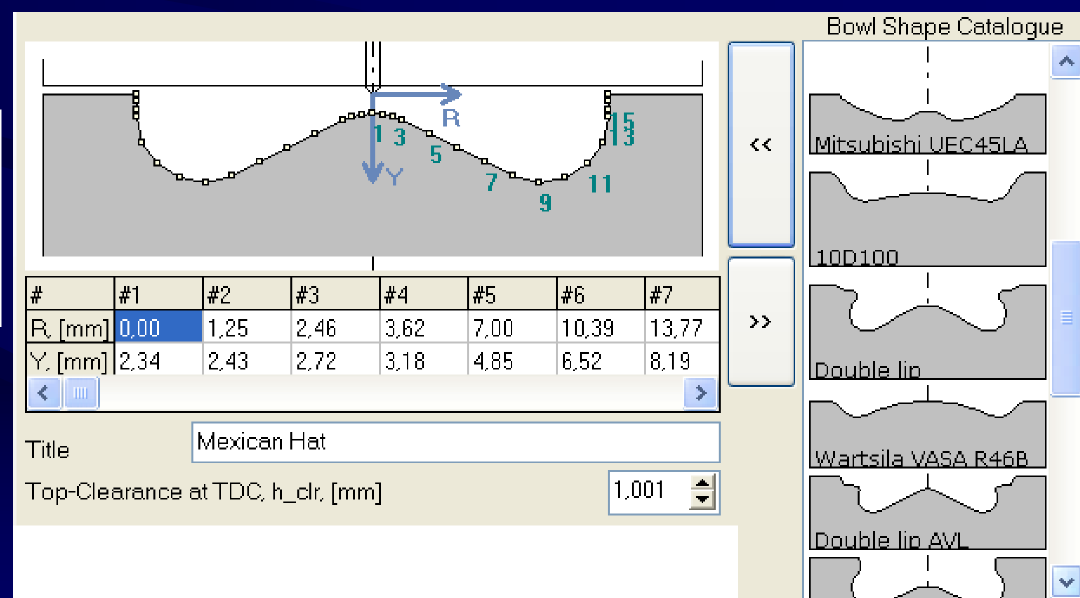



- Arbitrary piston bowl shape.



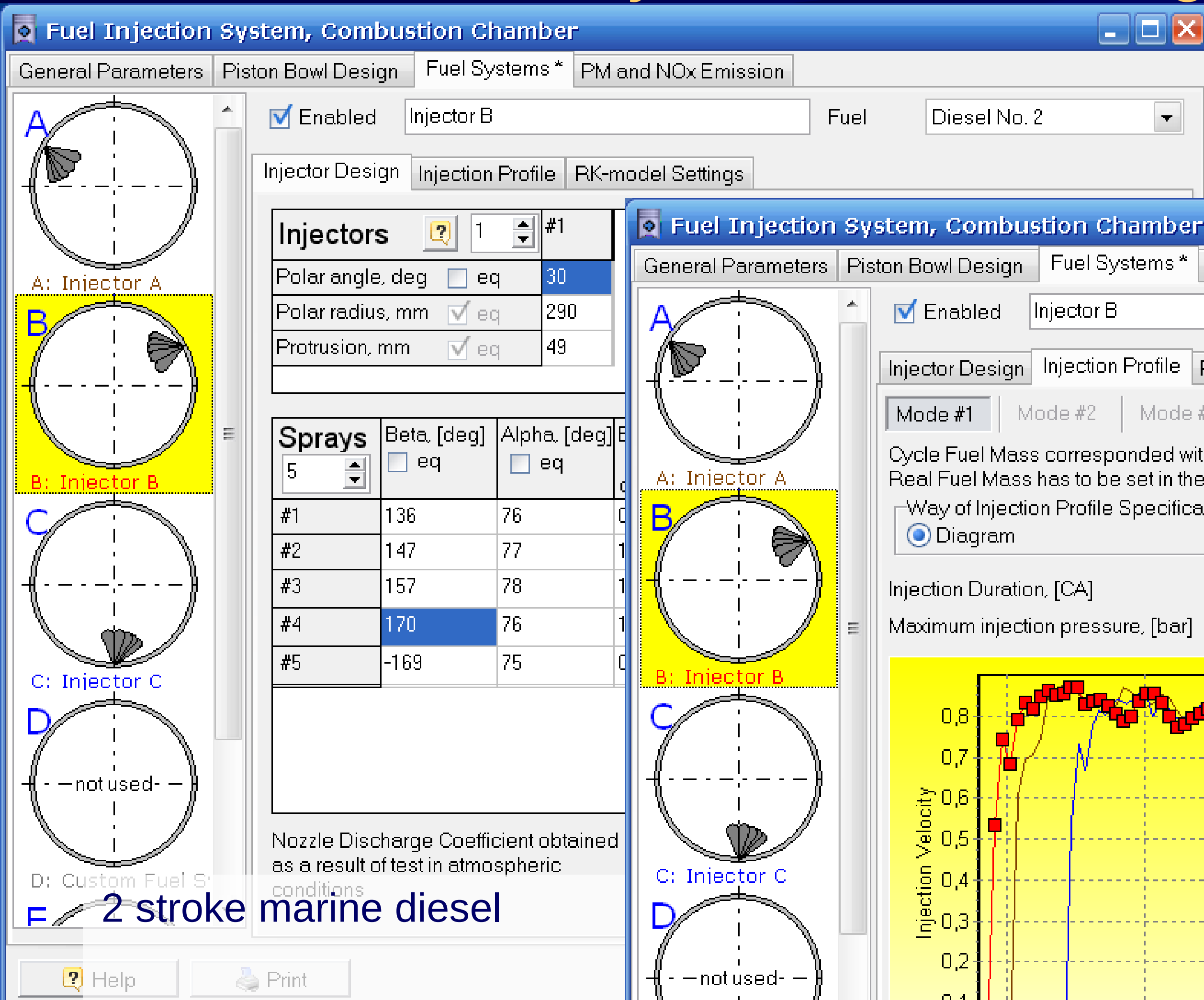

- Arbitrary sprays configuration.



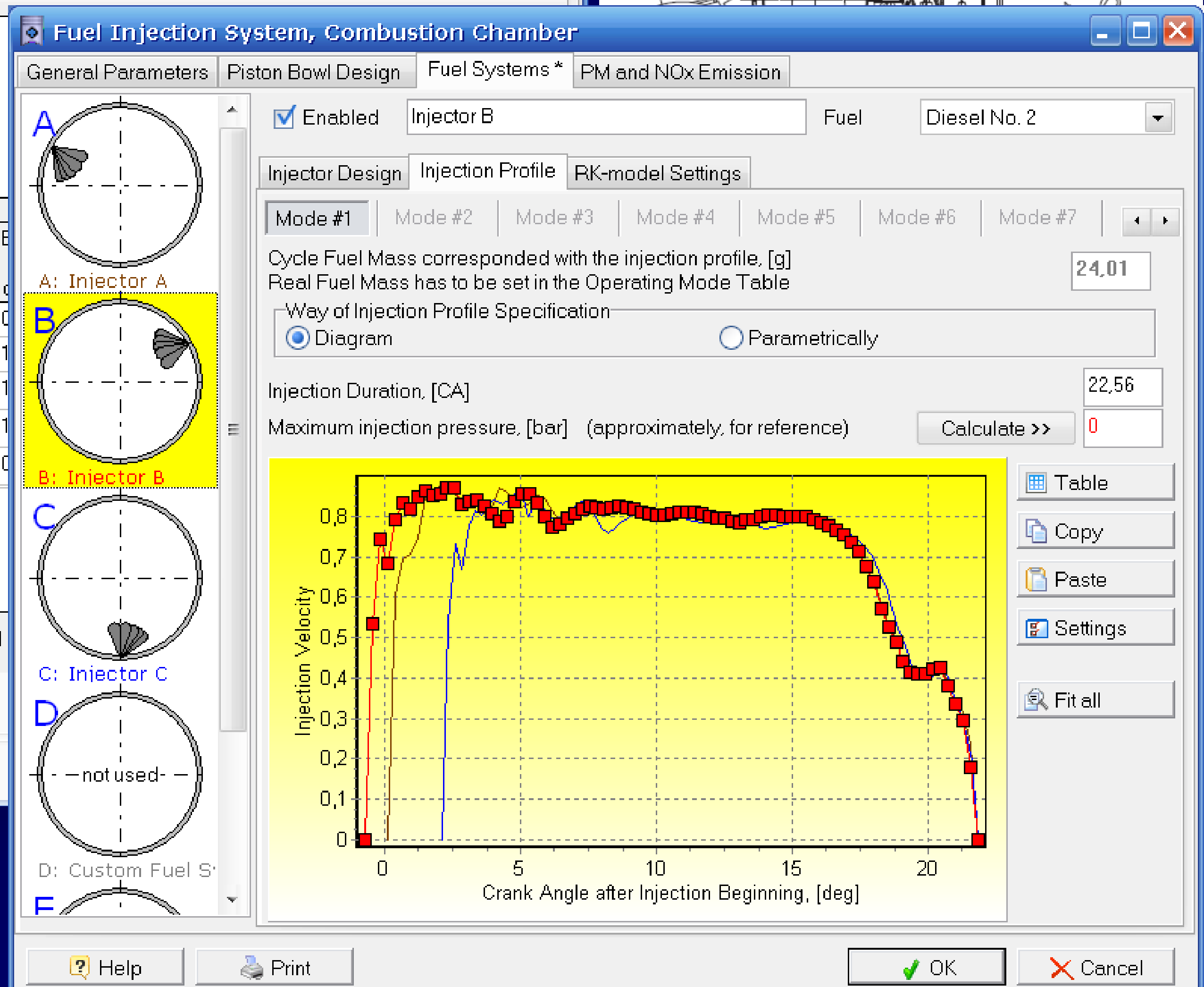




Data base of piston bowls is supported.

# Interface for specification of few Fuel Injection Systems in one engine

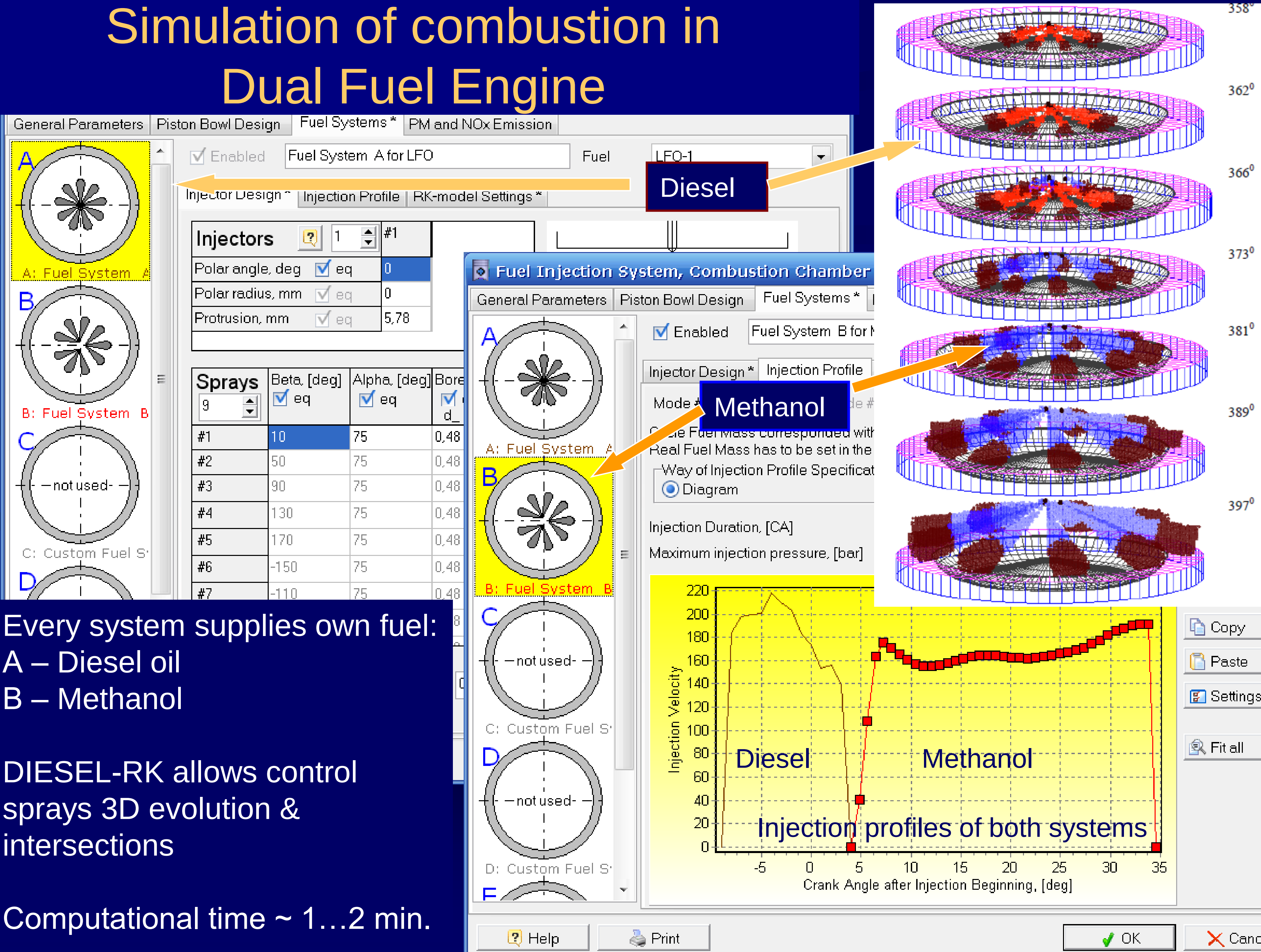



2 stroke marine diesel




Every injector has own injection profile

# Simulation of combustion in Dual Fuel Engine




Every system supplies own fuel:

A – Diesel oil

B – Methanol

DIESEL-RK allows control sprays 3D evolution & intersections

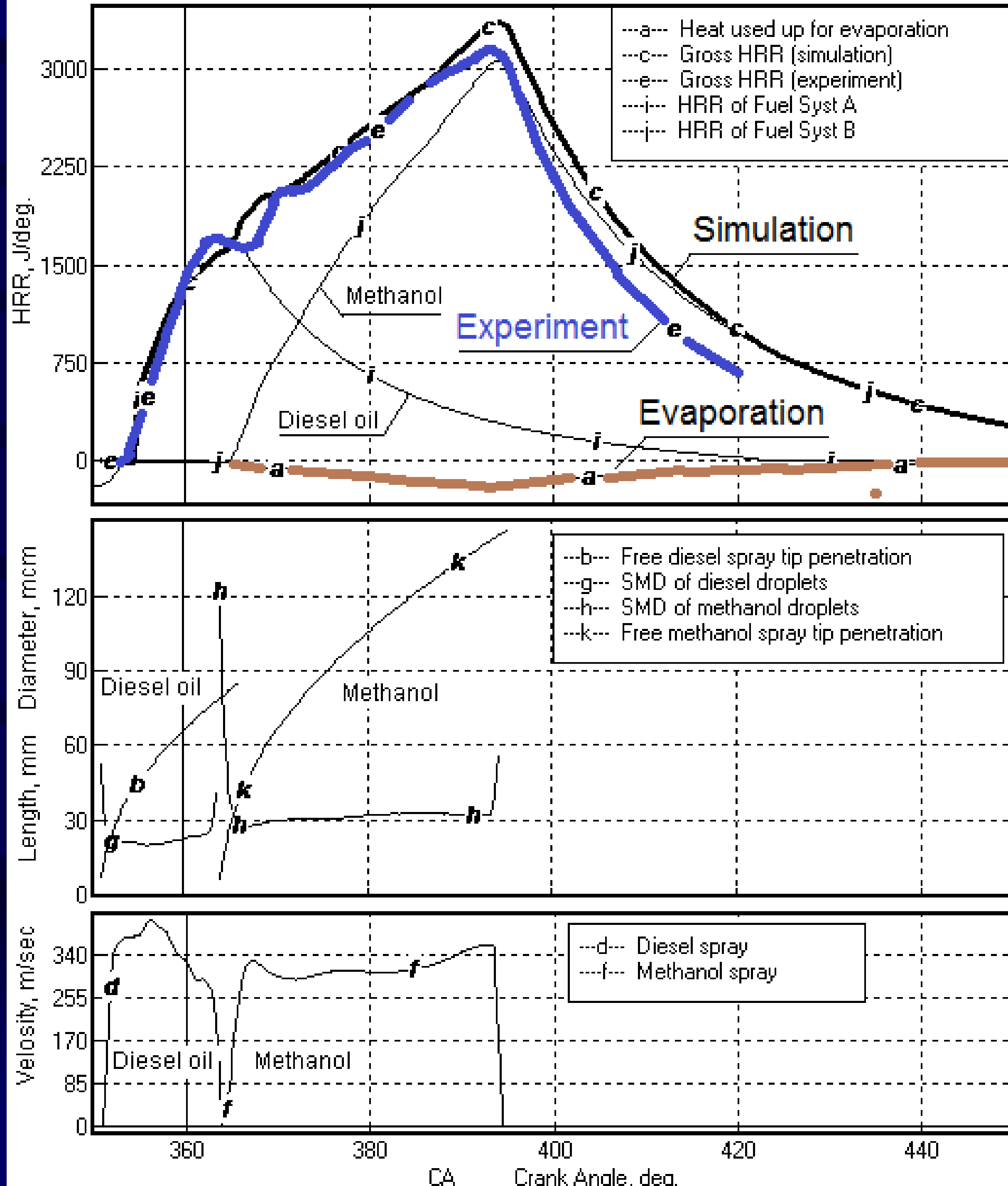
Computational time ~ 1…2 min.

# Simulation of combustion of Methanol in Dual Fuel Marine diesel W32

| | Experim. | Simulat. |
|---|---|---|
| *BMEP*, bar | 20.85 | 20.65 |
| $p_{max}$, бар | 160 | 164 |

Spray tip penetration [mm]
SMD [micron]

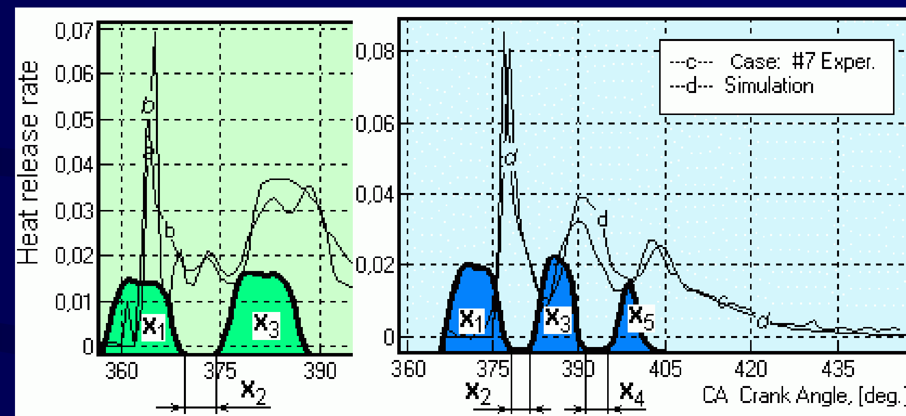
Injection profiles



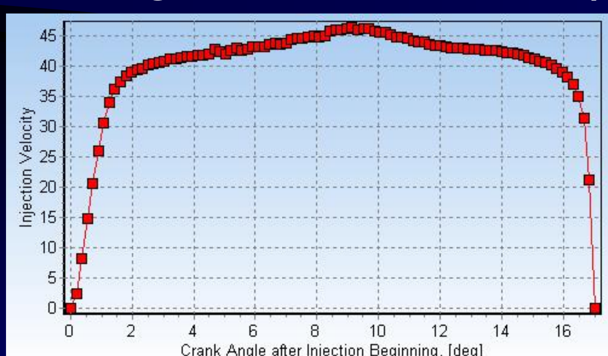
# DIESEL-RK capabilities

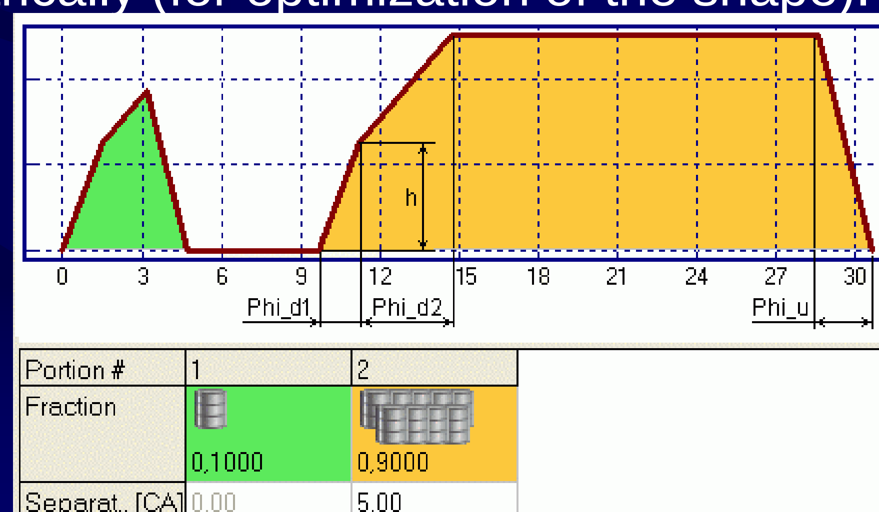
Full cycle thermodynamic engine simulation tool DIESEL-RK has following features for combustion optimization:

-Any multiple injection strategy.




- Injection profile may be specified:
  - as diagram;
  - parametrically (for optimization of the shape).




- Effect of high injection pressure.

# Soot formation model

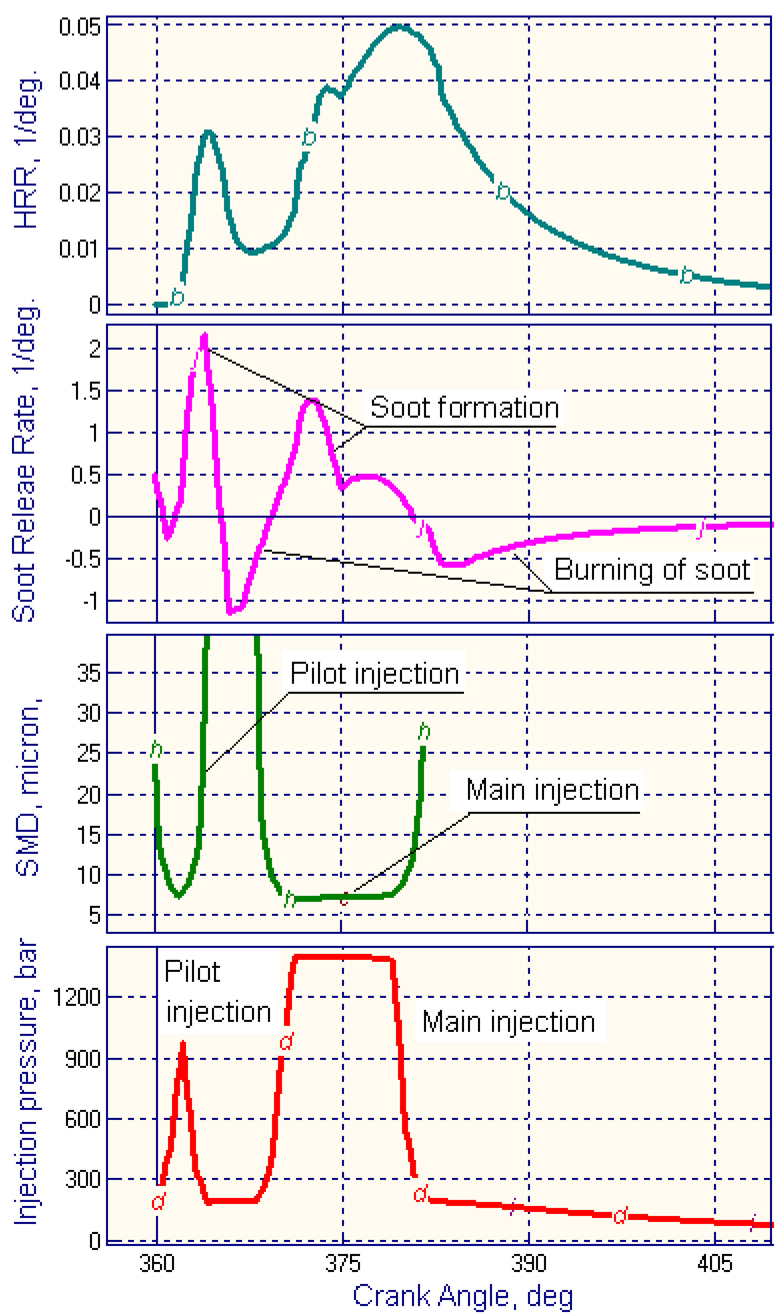
Phenomenological simulation method takes into account features of sprayed fuel burning. It is assumed, the soot is formed mainly by two ways:

- As a result of chain destructive transformation of molecules of fuel diffusing from the surface of drops to the front of a flame.
- Owing to high-temperature thermal polymerization and dehydrogenization of a vapor-liquid core of evaporating drops.

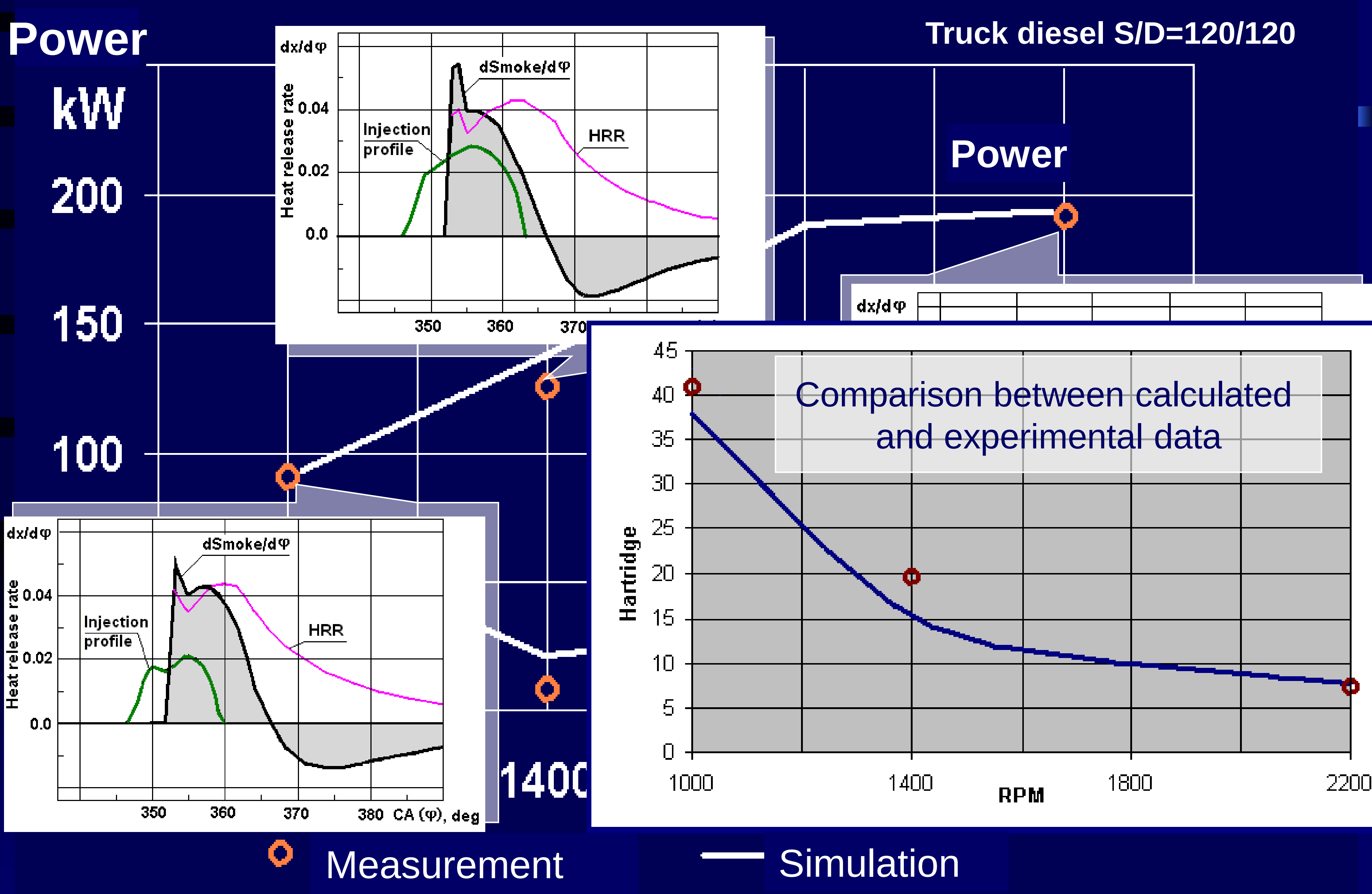
In parallel to this, the process of burning of soot particles and reduction of their volumetric concentration owing to expansion occurs.

Sauter Mean Diameter (SMD) of droplets is calculating during injection of every portion of multiple injection. Evaporation constants are calculated as functions of pressure and temperature of zones.

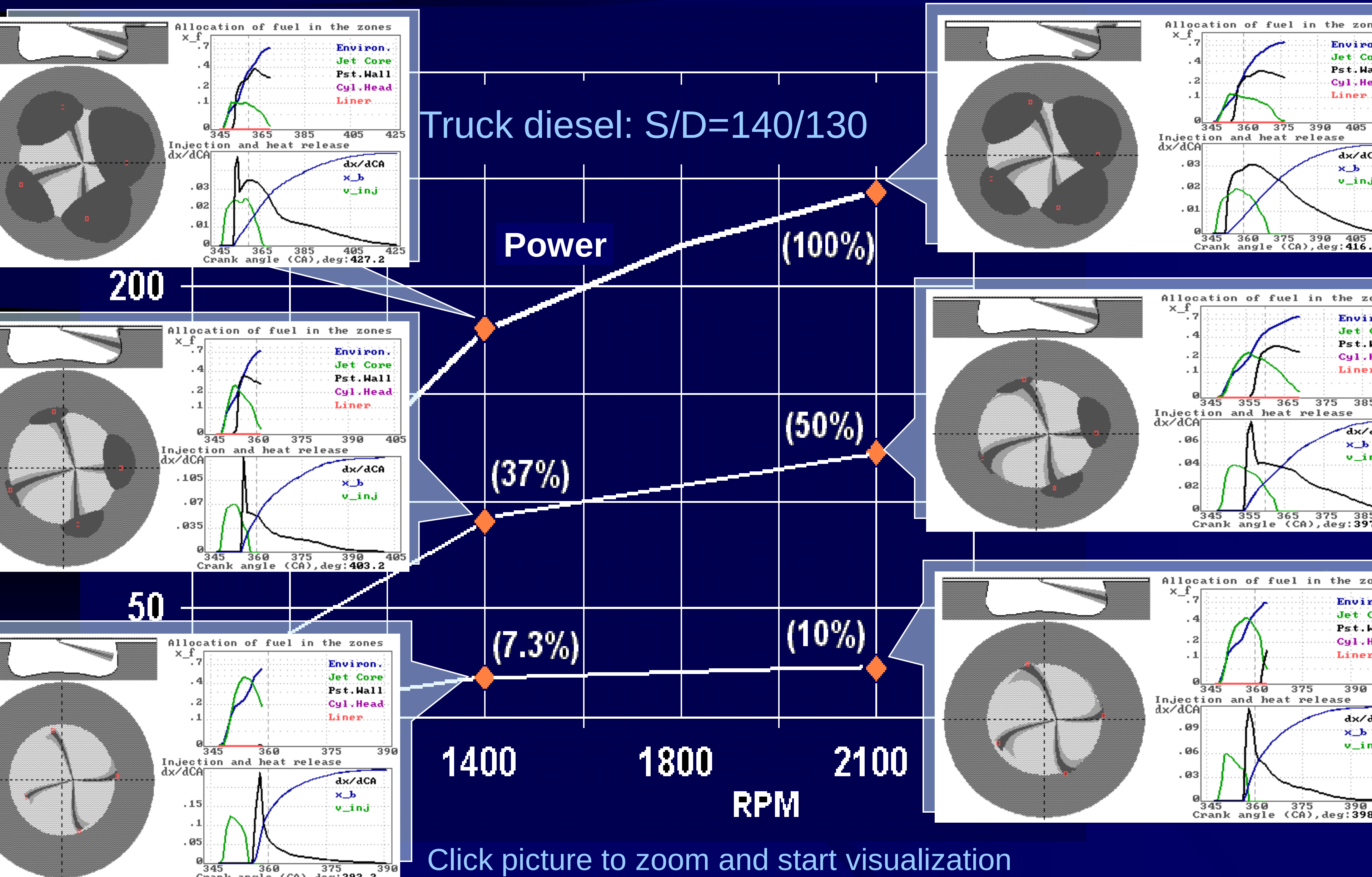
Diagrams show soot formation in z-engine at Max Torque point @1500 RPM having split injection: Pilot injection is 15% and sepatation is 4 deg. Injection pressure is a pressure before nozzles.



# Simulation of soot emission in the diesel over the whole speed range



# Illustration of high accuracy of ICE simulation over the whole operating range (1)

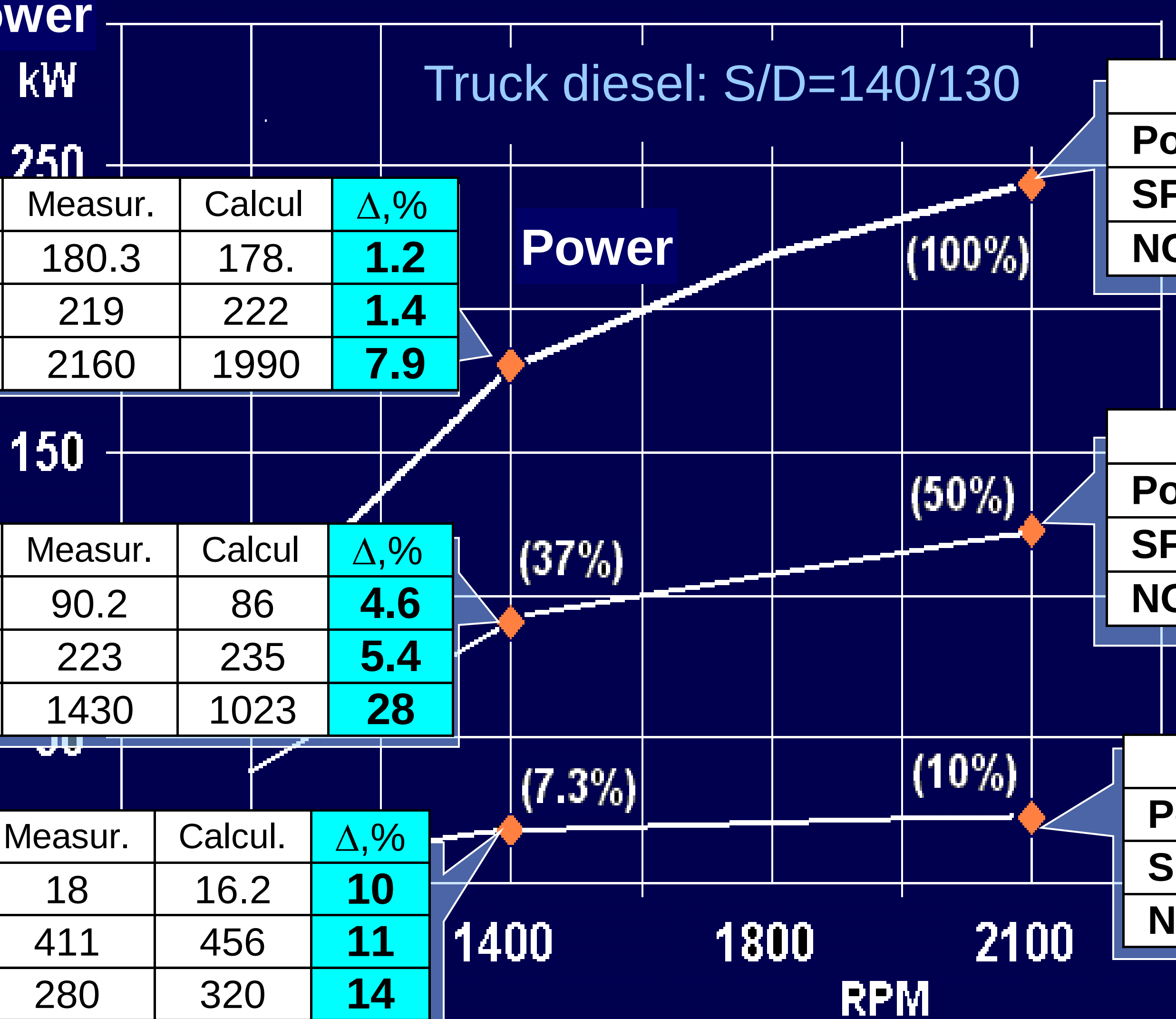



Click picture to zoom and start visualization

# Illustration of high accuracy of ICE simulation over the whole operating range (2)

Comparison between calculated and experimental data

Δ is the relative error




| | Measur. | Calcul | Δ,% |
|---|---|---|---|
| Pow | 180.3 | 178. | 1.2 |
| SFC | 219 | 222 | 1.4 |
| NOx | 2160 | 1990 | 7.9 |

| | Measur. | Calcul | Δ,% |
|---|---|---|---|
| Pow | 90.2 | 86 | 4.6 |
| SFC | 223 | 235 | 5.4 |
| NOx | 1430 | 1023 | 28 |

| | Measur. | Calcul. | Δ,% |
|---|---|---|---|
| Pow | 18 | 16.2 | 10 |
| SFC | 411 | 456 | 11 |
| NOx | 280 | 320 | 14 |

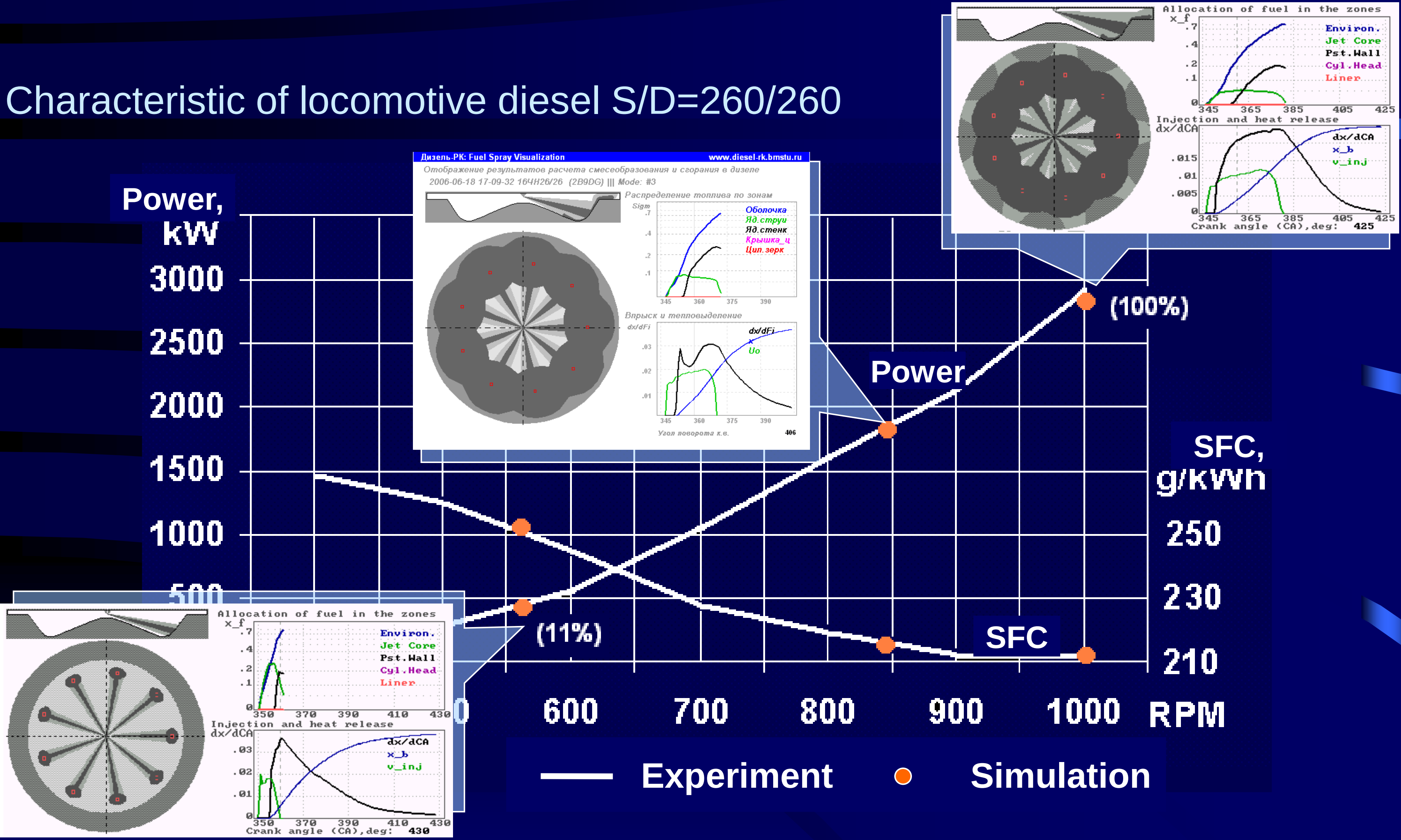
| | Measur. | Calcul. | Δ,% |
|---|---|---|---|
| Pow | 244.3 | 252 | 3.1 |
| SFC | 240 | 232 | 3.3 |
| NOx | 1920 | 1869 | 2.6 |

| | Measur. | Calcul. | Δ,% |
|---|---|---|---|
| Pow | 122.2 | 122. | 0 |
| SFC | 258 | 258 | 0 |
| NOx | 980 | 930 | 5.1 |

| | Measur. | Calcul. | Δ,% |
|---|---|---|---|
| Pow | 24.4 | 25.1 | 2.9 |
| SFC | 577 | 560 | 2.9 |
| NOx | 240 | 260 | 8.3 |

# Illustration of high accuracy of ICE simulation over the whole operating range (3)

Characteristic of locomotive diesel S/D=260/260




Click picture to zoom and start visualization

# Illustration of high accuracy of ICE simulation over the whole operating range (4)

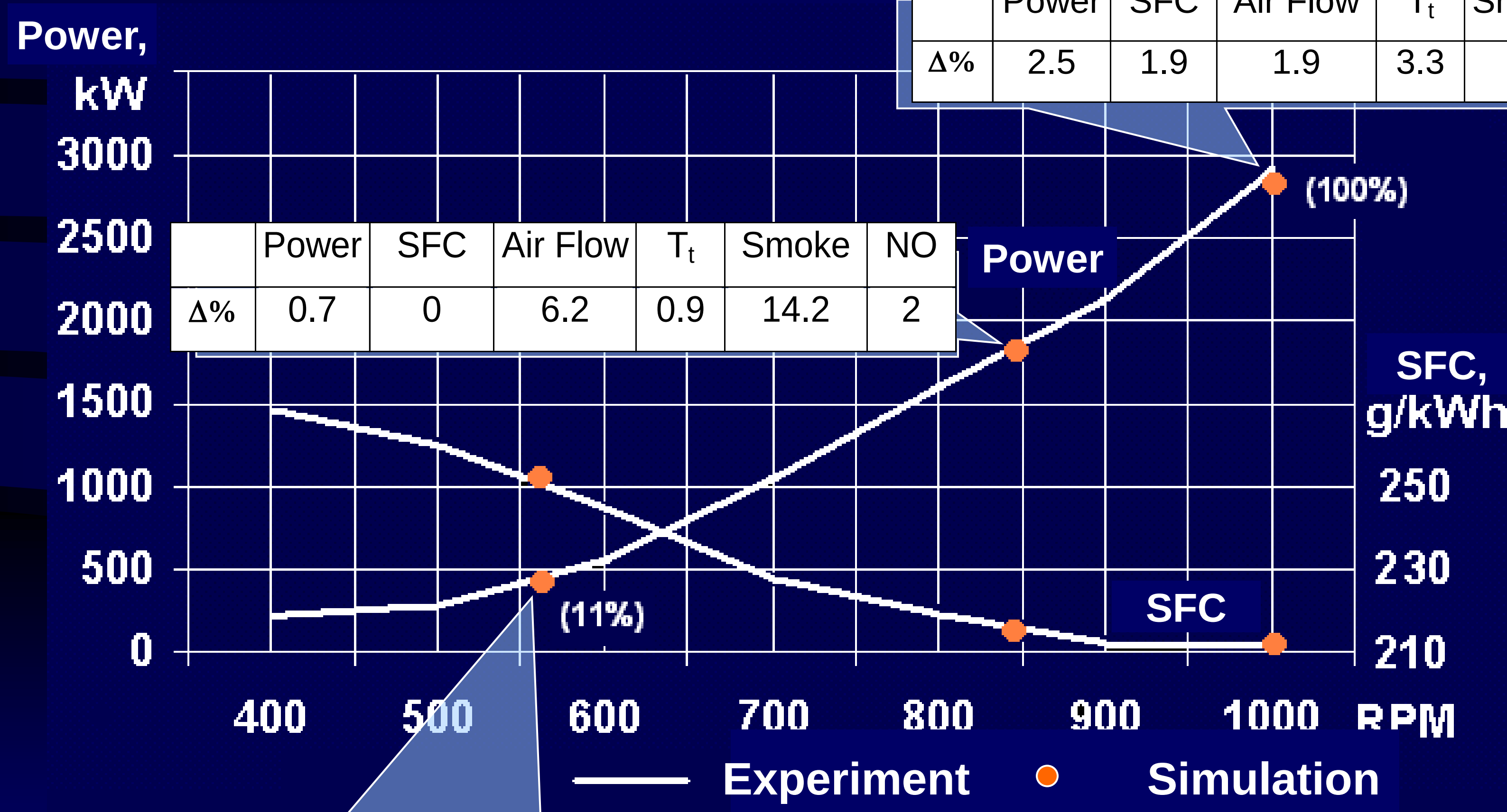
Comparison between calculated and experimental data

Characteristic of locomotive diesel S/D=260/260

Δ is the relative error.

| | Power | SFC | Air Flow | $T_t$ | Smoke | NO |
|---|---|---|---|---|---|---|
| Δ% | 2.5 | 1.9 | 1.9 | 3.3 | 0 | 0.6 |

| | Power | SFC | Air Flow | $T_t$ | Smoke | NO |
|---|---|---|---|---|---|---|
| Δ% | 0.7 | 0 | 6.2 | 0.9 | 14.2 | 2 |




| | Power | SFC | Air Flow | $T_t$ | Smoke | NO |
|---|---|---|---|---|---|---|
| Δ% | 3.6 | 3.5 | 1 | 1.2 | 7.1 | 0.7 |

Air Flow is the Air flow rate;
$T_t$ is Turbine inlet temperature;
Smoke is the Bosch smoke number.

$l_{wj} = K_j \, B_{sw}^{0.5} \, \tau_w^{0.5}$

# Advanced NOx Formation Model

## - Detail Kinetic Mechanism

for advanced diesel engines:

- with **Multiple Injection** or / and with high **EGR**
- working on alternative fuels: **DME, Biofuel**

The detail kinetic mechanism consists of two blocks:
- initial disintegration of a fuel molecule, consisting of **40 reactions** with participation of **10 species**;
- the detail kinetic mechanism of methane oxidation and NOx formation, consisting of **199 reactions** and **33 species**.

## - Thermal Zeldovich's mechanism

for conventional diesel engines

- Temperature in a zone of combustion is defined by zone model.
- On each step the equilibrium composition of **18 species** is defined in a zone of combustion.
- The calculation of NOx formation is carried out with the kinetic equation.

O, $O_2$, $O_3$, H, $H_2$, OH, $H_2O$, C, CO, $CO_2$, $CH_4$, N, $N_2$, **NO, $NO_2$**, $NH_3$, $HNO_3$, HCN

$l_{wj} = K_j B_{sw}^{0.5} \tau_w^{0.5}$

# Advanced NOx Formation Model

- **Thermal Zeldovich's mechanism** can not be used for engines with large EGR.
- **Detail Kinetic Mechanism** (Basevich's scheme)

DKM is intended for engines:

- with **Multiple Injection** or / and with massive **EGR** or/and with **PCCI**;
- working on alternative fuels: **DME, Biofuel, etc.**

The detail kinetic mechanism consists of two blocks:

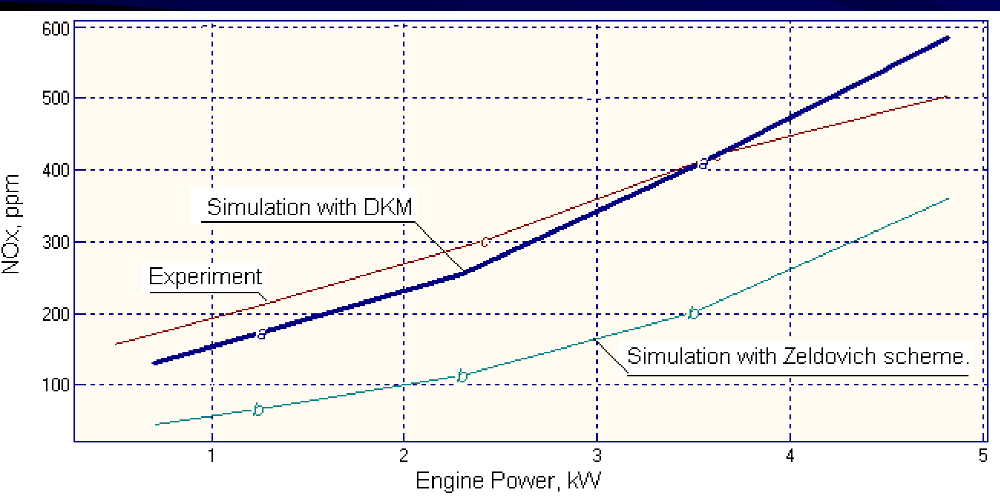
1) The Initial disintegration of a fuel molecule, consisting of **40 reactions** with **10 species**;
2) The detail kinetic mechanism of methane oxidation and NOx formation, consisting of **199 reactions** with **33 species**.

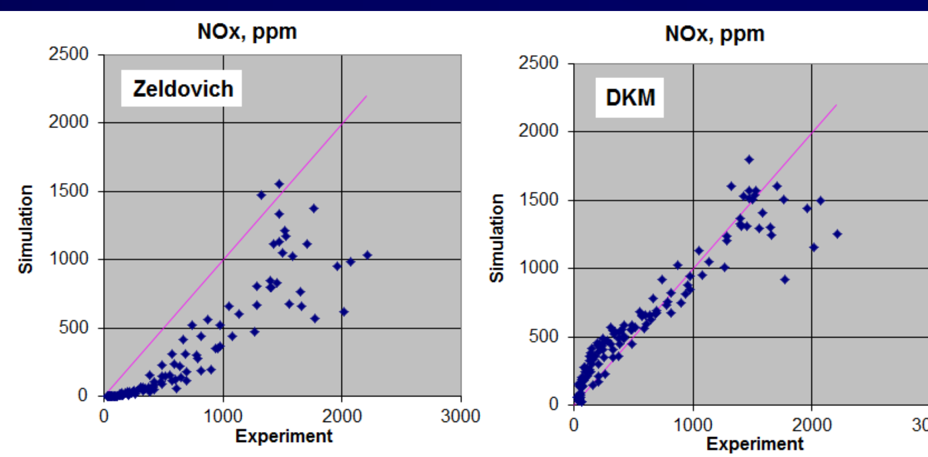
- Temperature in a zone of combustion is defined by zone model.

Measured NOx and simulated NOx with Zeldovich and DKM

a) for 1 cyl. diesel engine S/D=66/82 mm) and 3600 RPM.

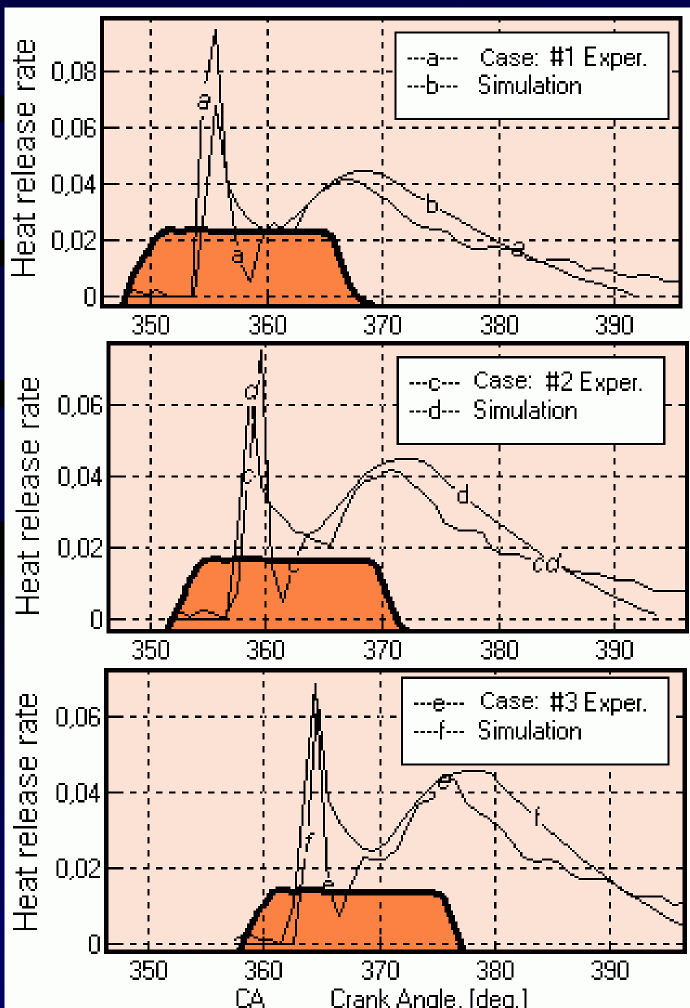
b) 4cyl. 2 liters light duty diesel with max BMEP=26 bar (massive EGR)

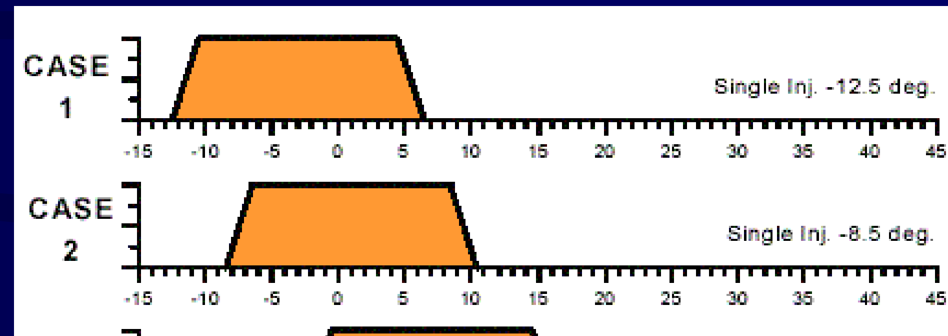


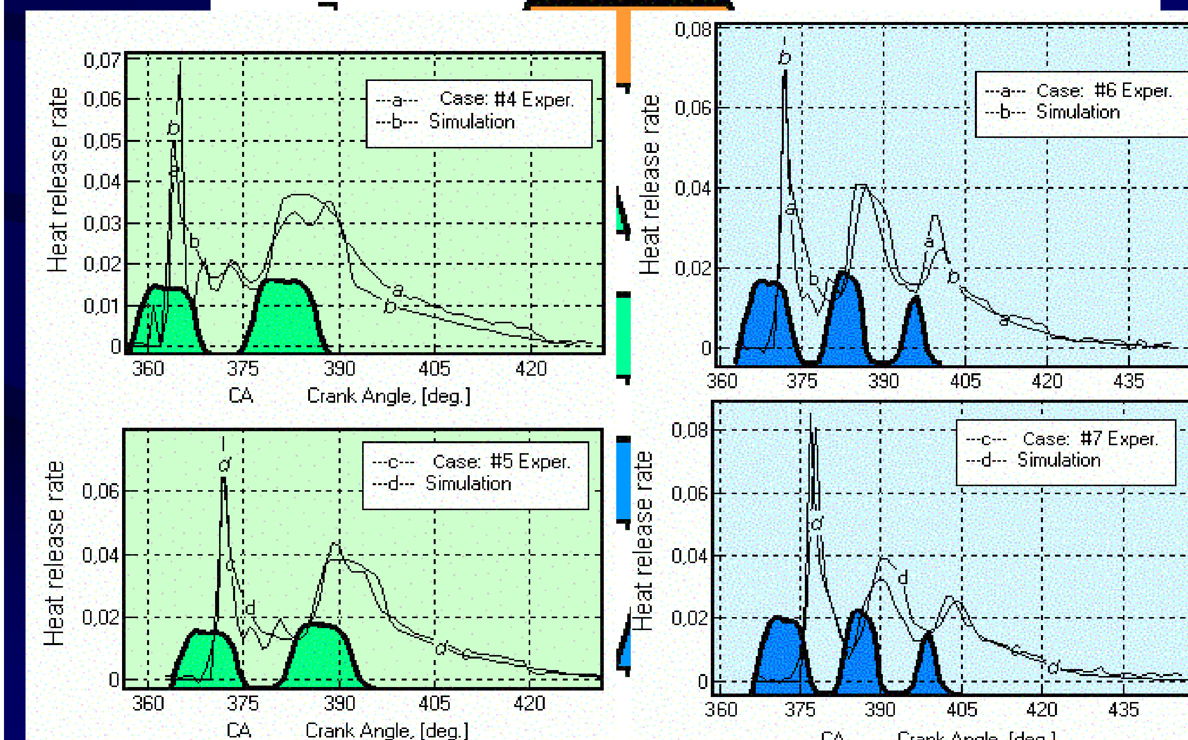



# Simulation of combustion in diesel with different strategies of fuel injection

**Comparison between calculated data and experimental ones published by M. Bakenhus & R.Reitz: SAE pap. N 1999-01-1112**



# Simulation of NOx formation in diesel with different strategies of fuel injection

**Comparison calculated data with experimental ones published by M. Bakenhus & R.Reitz: SAE pap. N 1999-01-1112**

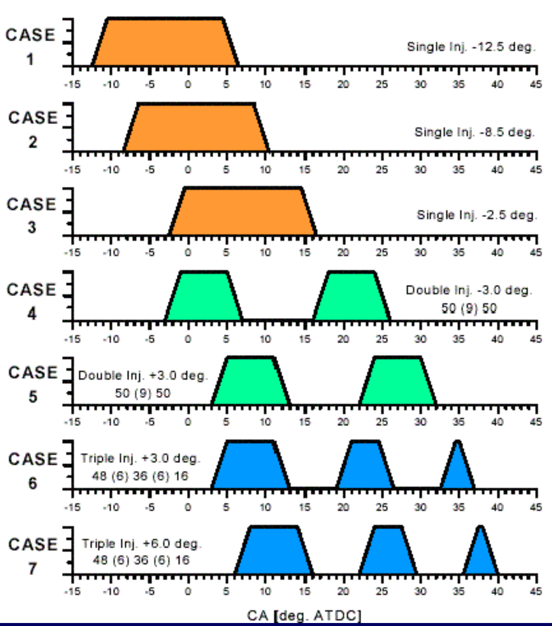
**Caterpillar 3401**

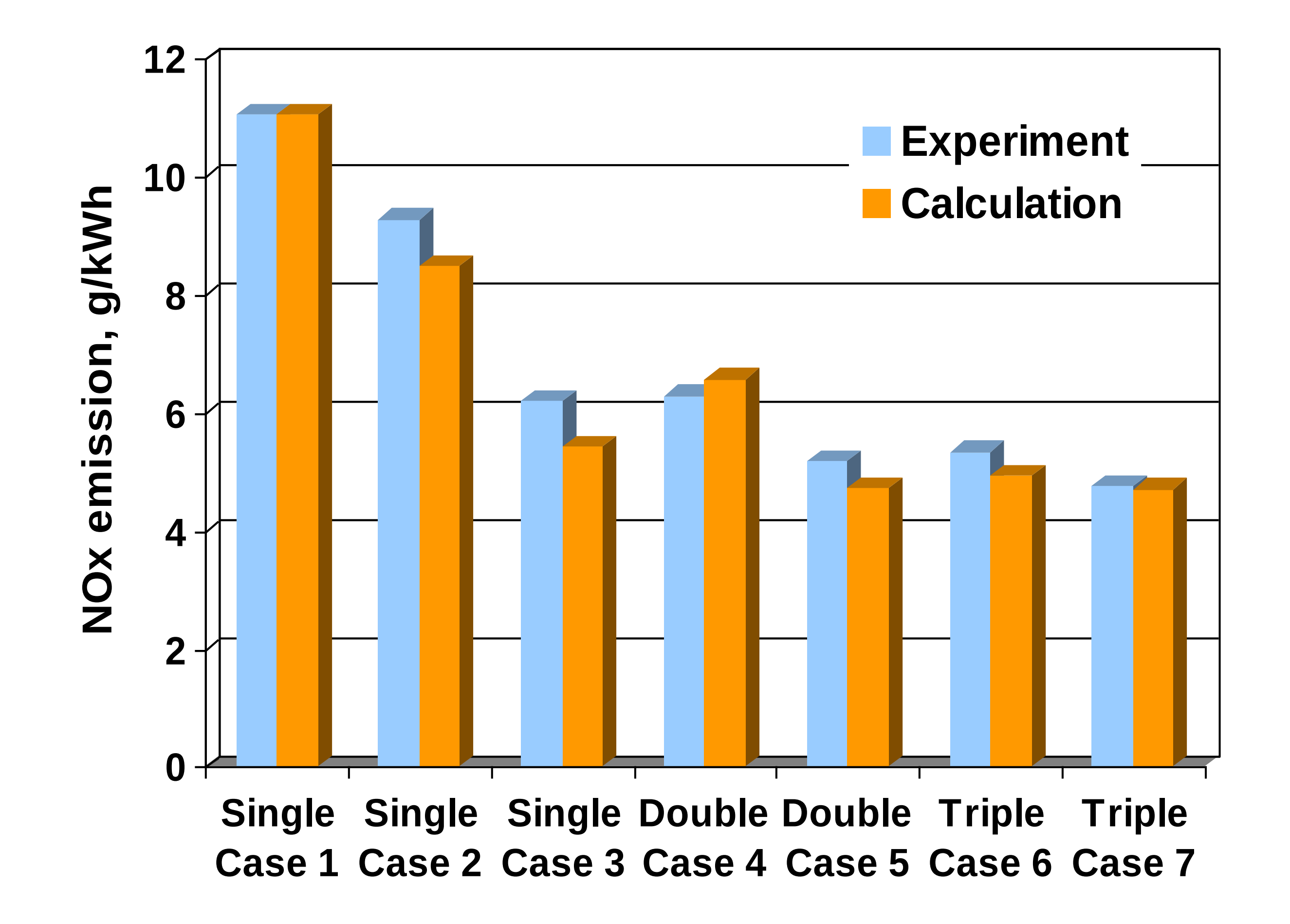
D/S=137/165; ε=16.5

BMEP=10 bars

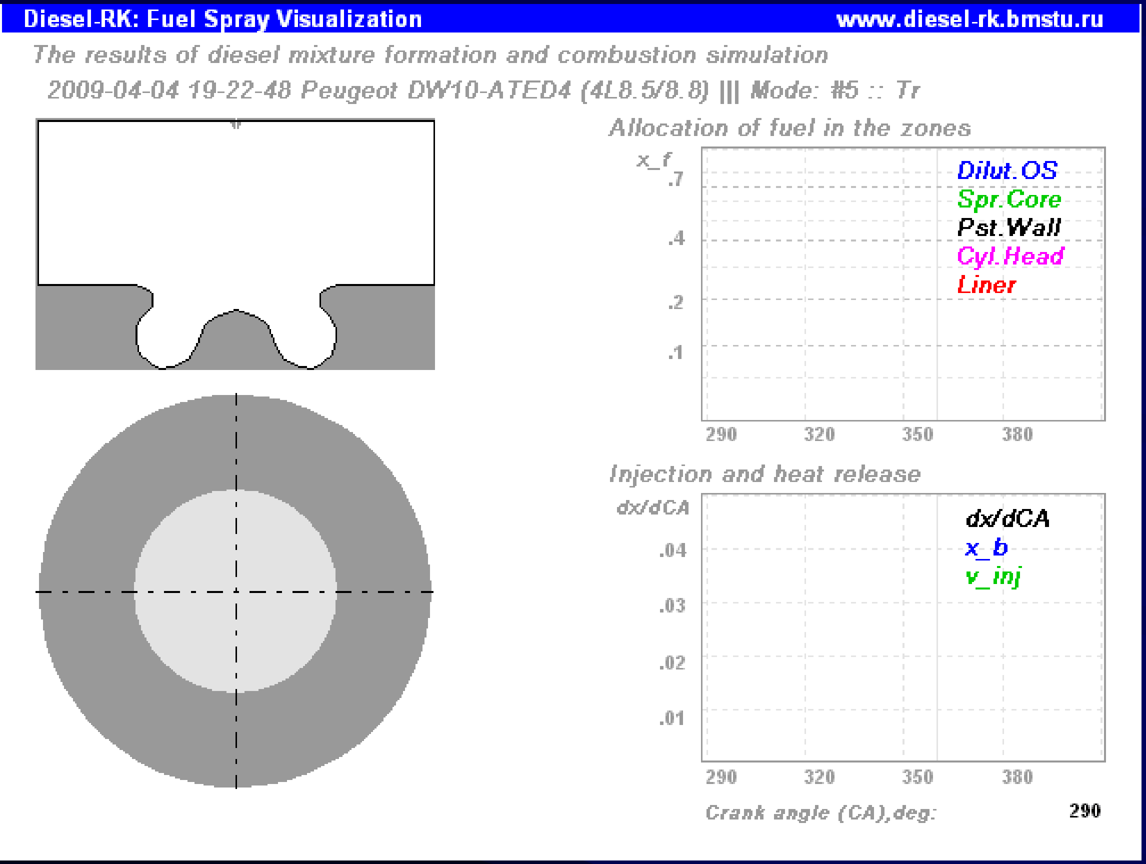
RPM=1600,

Injector: 6x0.259x125



# PCCI modeling




**RPM=2600  BMEP=8.7 bar**

Engine:
Peugeot DW10-ATED4
D = 85 mm  S = 88 mm
RPMnom = 4000;
injector: 6 x 0.14

Triple pilot injection;
pilots fuel fraction: 28%

Experimental data were published by:
Gary D. Neely, Shizuo Sasaki and Jeffrey A. Leet "Experimental Investigation of PCCI-DI Combustion on emissions in a Light-Duty Diesel Engine" SAE Pap N 2004-01-0121, 2004

# PCCI modeling

It is possible to define duration and fraction of each pilot to avoid the hitting of the fuel on the liner

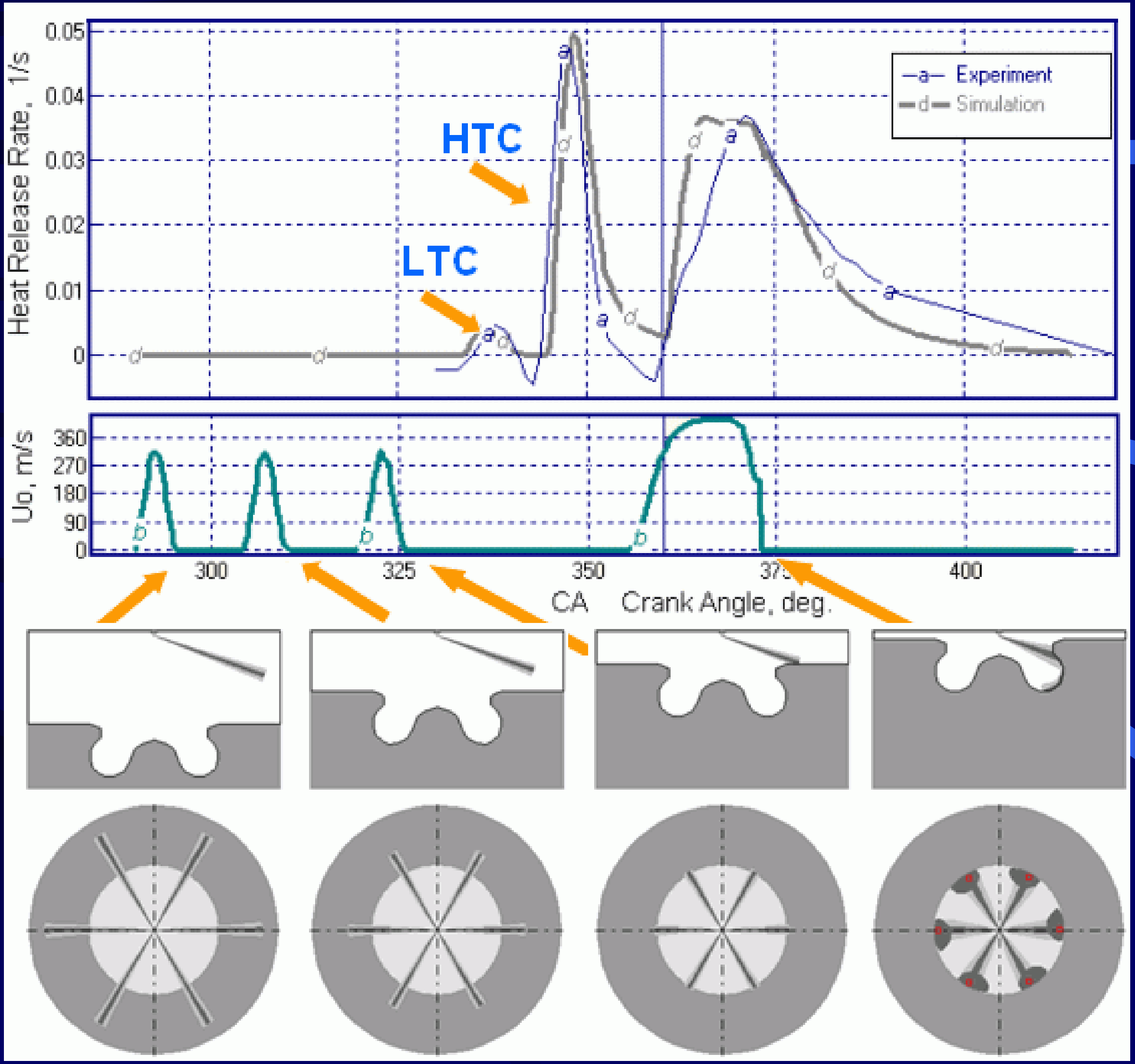
**Peugeot DW10-ATED4**

**(4L8.5/8.8)**

**RPM=2600**

*LTC: Low Temperature Combustion*

*HTC: High Temperature Combustion*



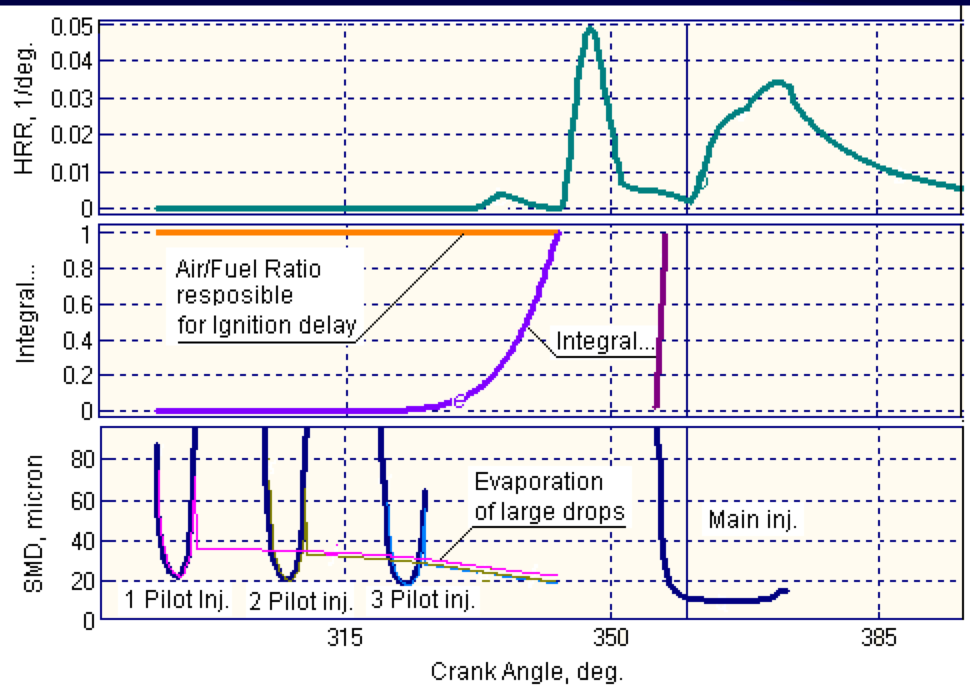
# PCCI modeling

If Large Drops injected at the end of every portion have not enough time to be evaporated completely the Air/Fuel eq. ratio being responsible for ignition delay is 1 (left diagram).

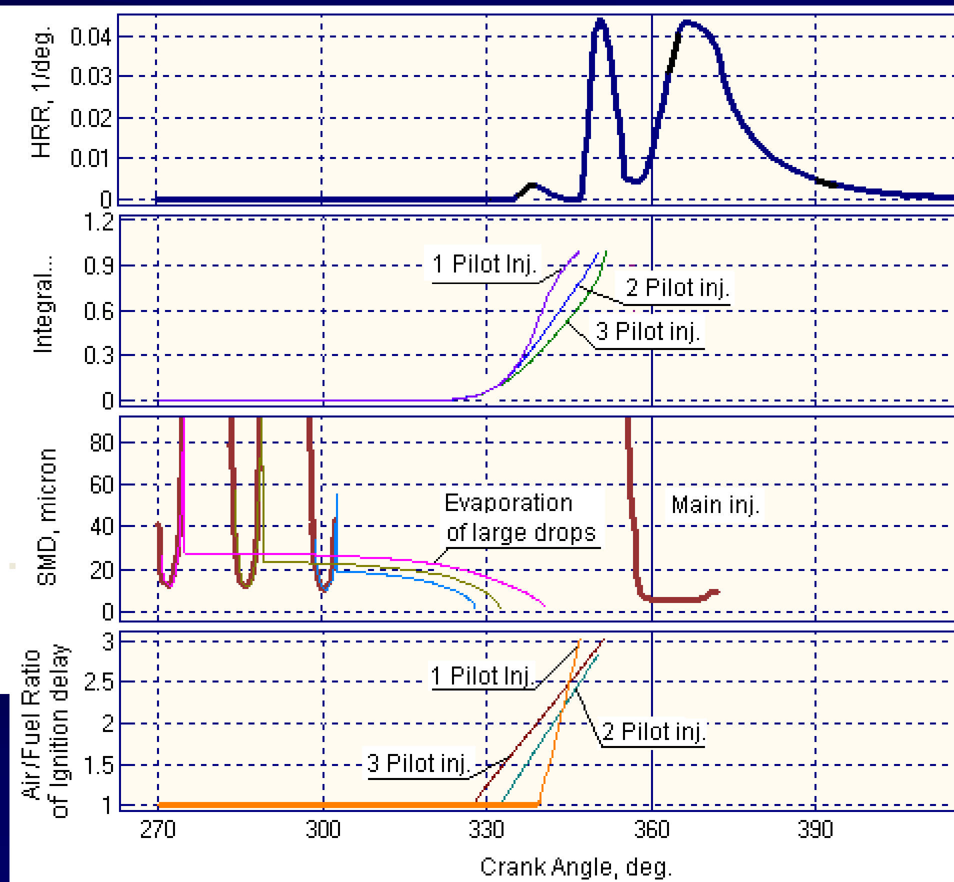
If the Large Drops are evaporated The Air/Fuel eq. ratio starts to grow up to total value being character for whole cylinder; it results in: preparation of fuel to selfignition slows down. First portion being ignited will have Integral reached 1 first.

**Peugeot DW10-ATED4 (4L8.5/8.8) RPM=2600; BMEP = 8.7 bar; Triple pilot: 28%**

*Injection timing : 70 deg .BTDC*




*Injection timing : 90 deg. BTDC*




*Livengood – Wu integral of Ignition Delay:*

$$\int_0^{\tau_i} \frac{d\tau}{\tau_{ign}} = 1$$

# PCCI modeling

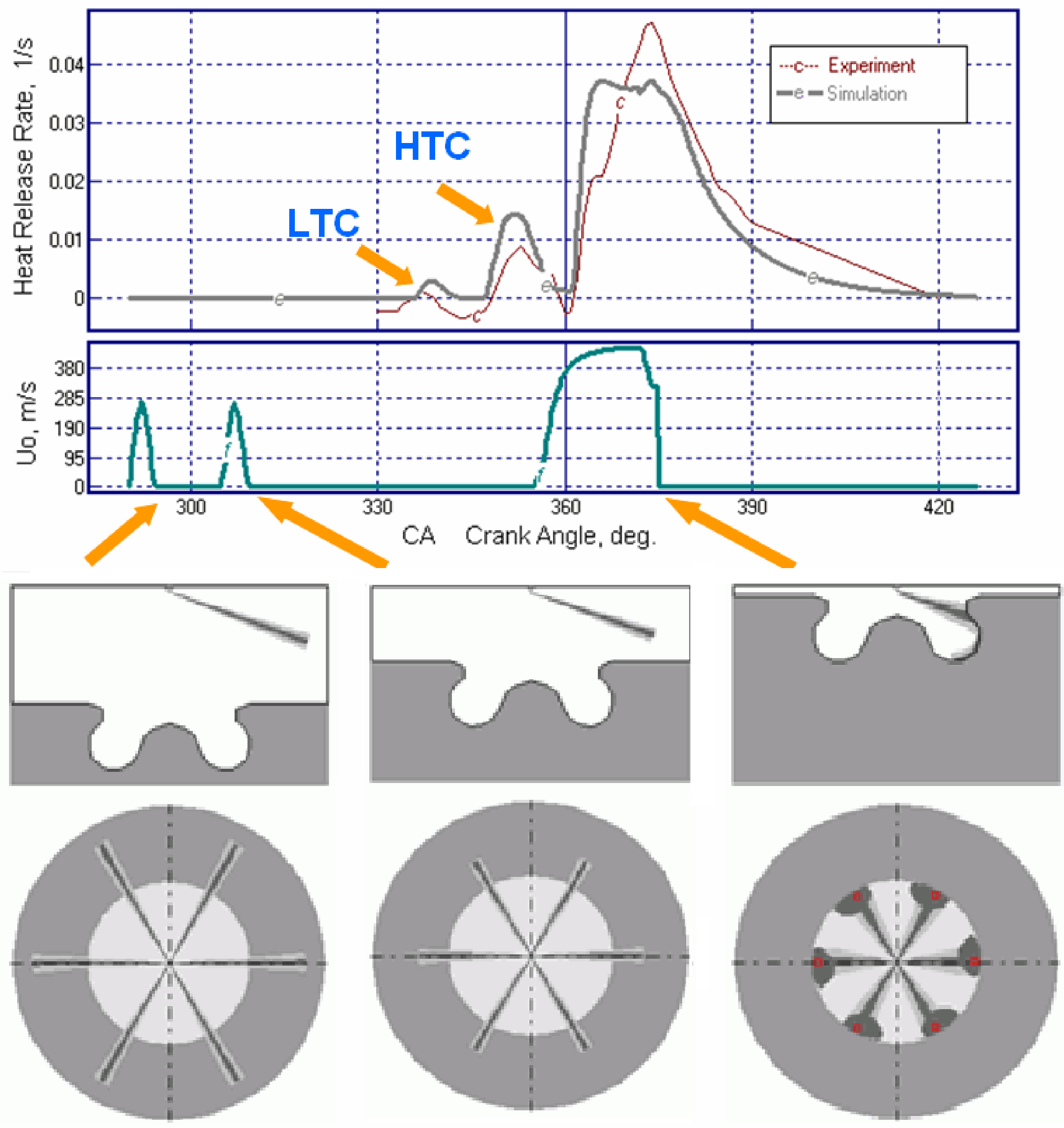
**Peugeot DW10-ATED4 (4L8.5/8.8)**

**RPM=2600**

**Double pilot 15%**

*LTC: Low Temperature Combustion*

*HTC: High Temperature Combustion*




Experimental data were published by:
Gary D. Neely, Shizuo Sasaki and Jeffrey A. Leet "Experimental Investigation of PCCI-DI Combustion on emissions in a Light-Duty Diesel Engine" SAE Pap N 2004-01-0121, 2004

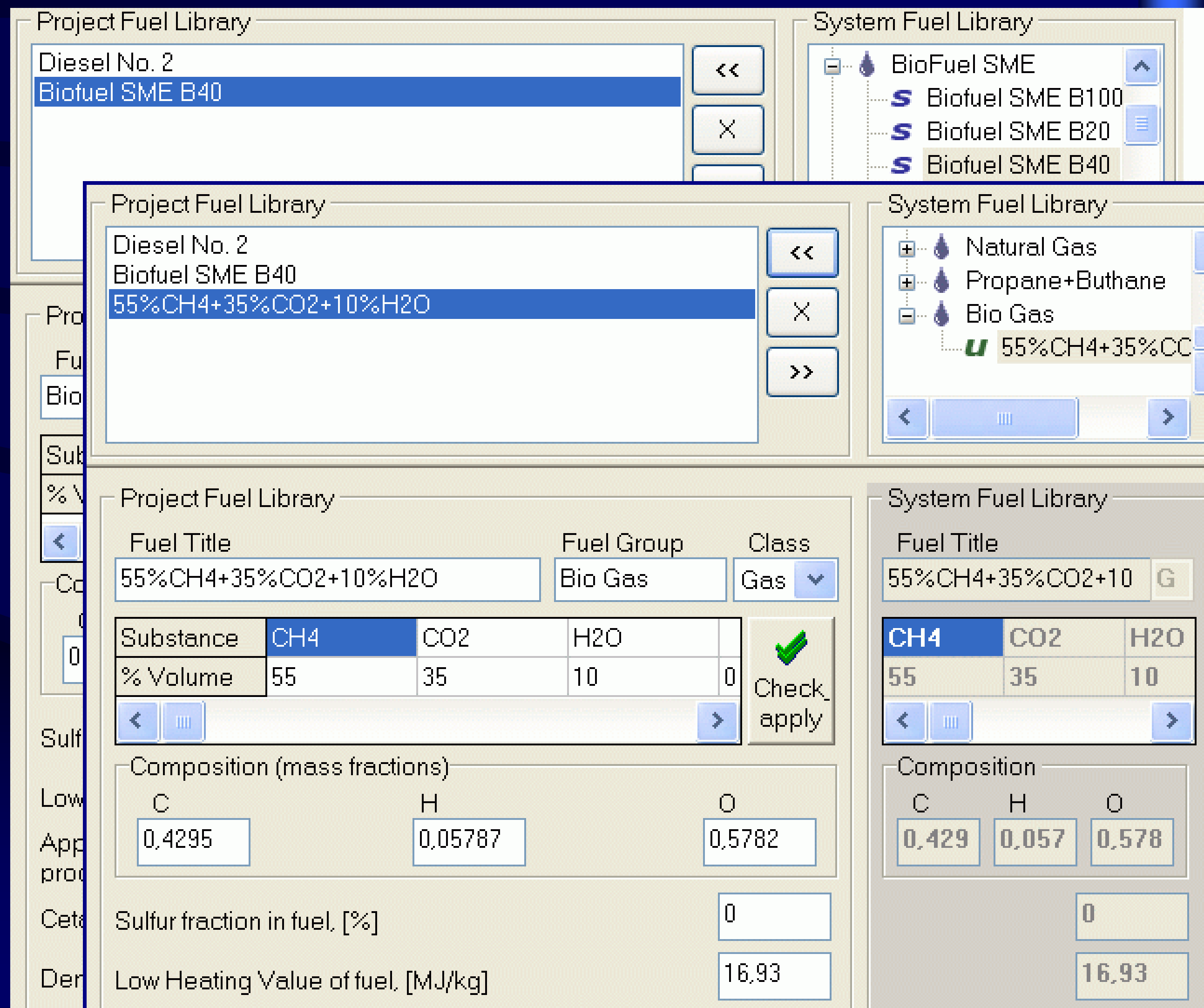
# Data base of fuels and Gas engines simulation

User can create own fuel and save one in the data base.
-- Blends of biofuels with diesel oil are supported.
-- Arbitrary mixed of gases are supported for gas engine. Properties of mixture are calculated automatically

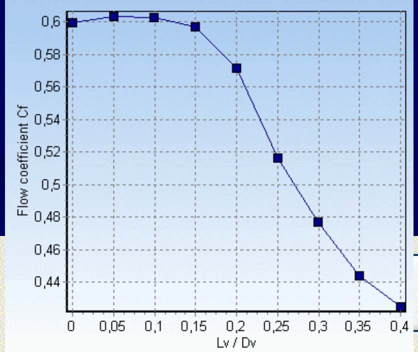
It is possible to set individual fuel for every operating mode. It allows presentation of engine parameters as function of fuel composition.

List of gases

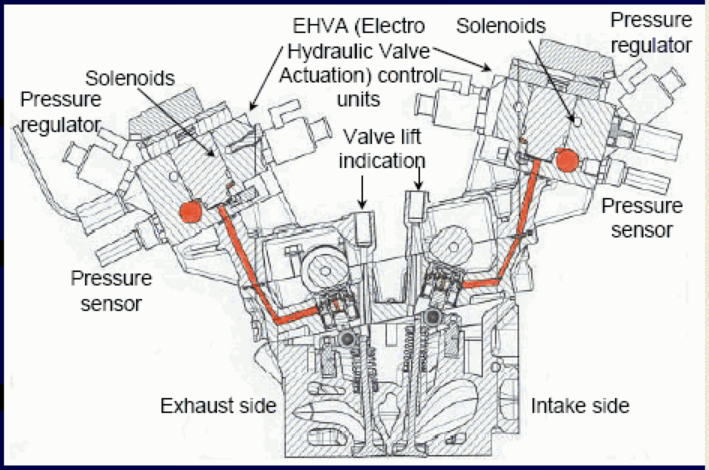
| | |
|---|---|
| H2 | Hydrogen |
| O2 | Oxygen |
| N2 | Nitrogen |
| H2O | Water Vapor |
| CO2 | Carbon Dioxide |
| CH4 | Methane |
| C2H6 | Ethane |
| C3H8 | Propane |
| C4H10 | Buthane |
| CH3OH | Methanol |
| CH3-O-CH3 | Dimethyl Ether |
| C2H5OH | Ethanol |

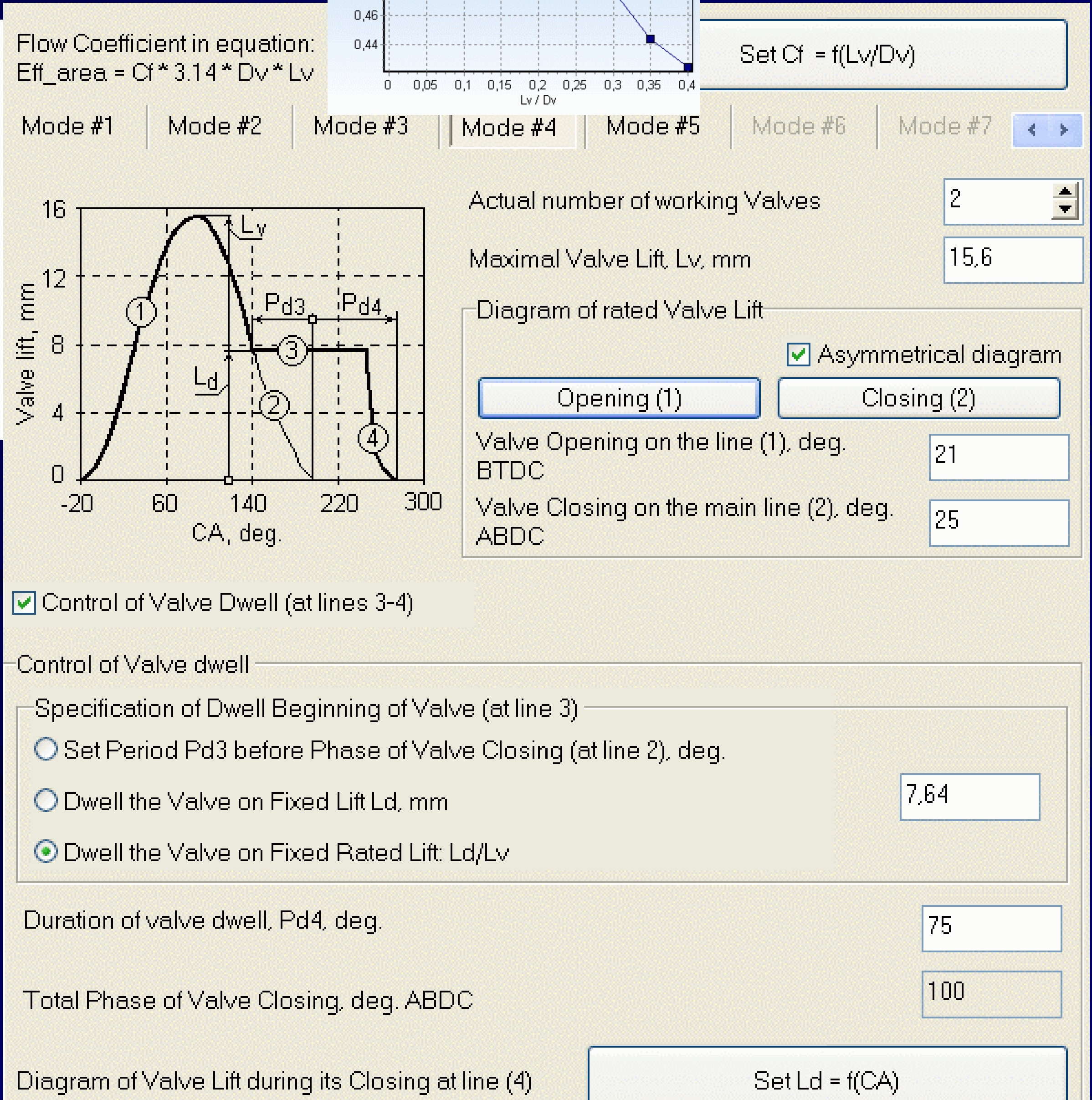


# Variable Valve Lift / Timing Analysis

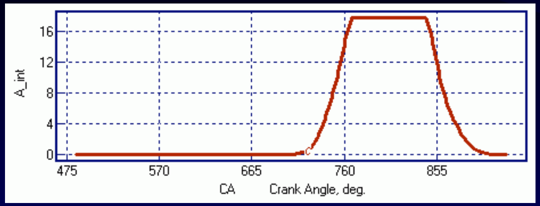


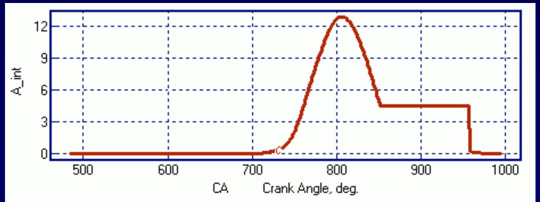

Flow Coefficient as a function of Valve Lift




Valve Lift Diagram with variable valve actuation can be set individually for every operating mode. Resulted Effective flow area diagrams:

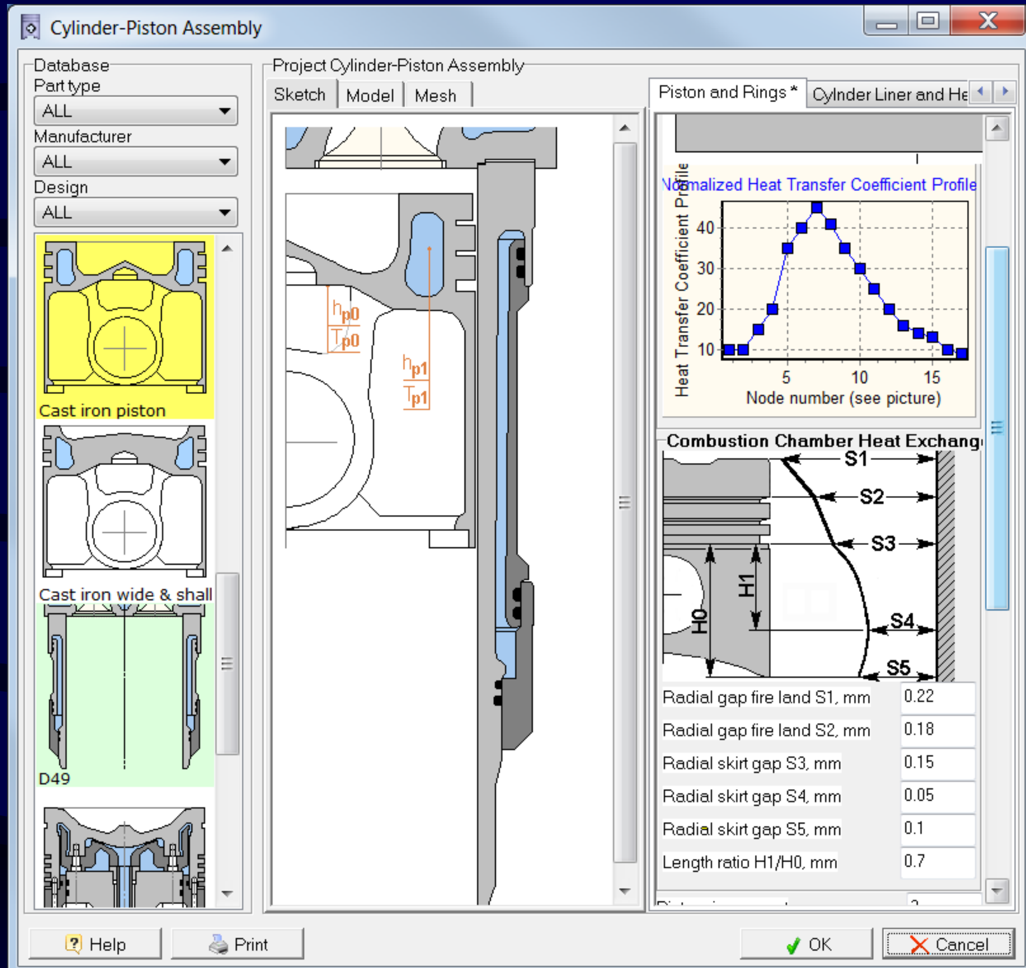


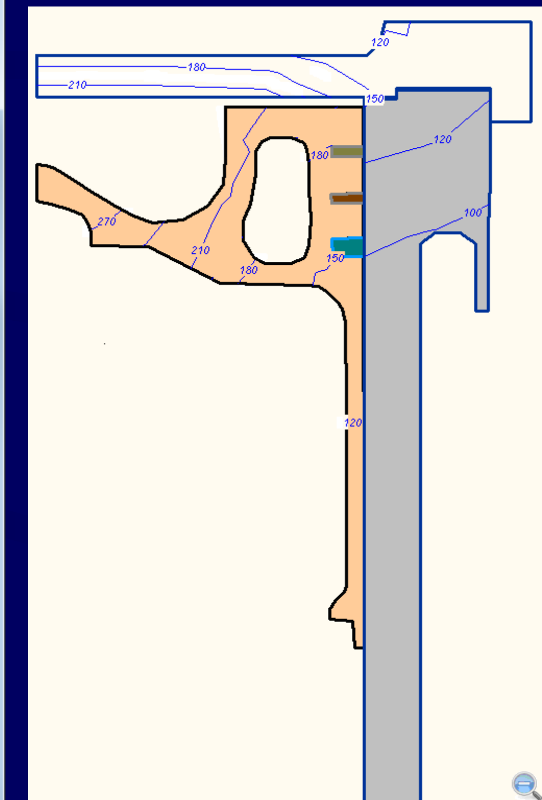
# Detail temperature fields of engine components

Account of walls local temperatures at in-cylinder processes simulation.

Simultaneous simulation of thermo-dynamic processes with **Finite Element Analysis**




Mesh is generated automatically




Data base of engine parts is included

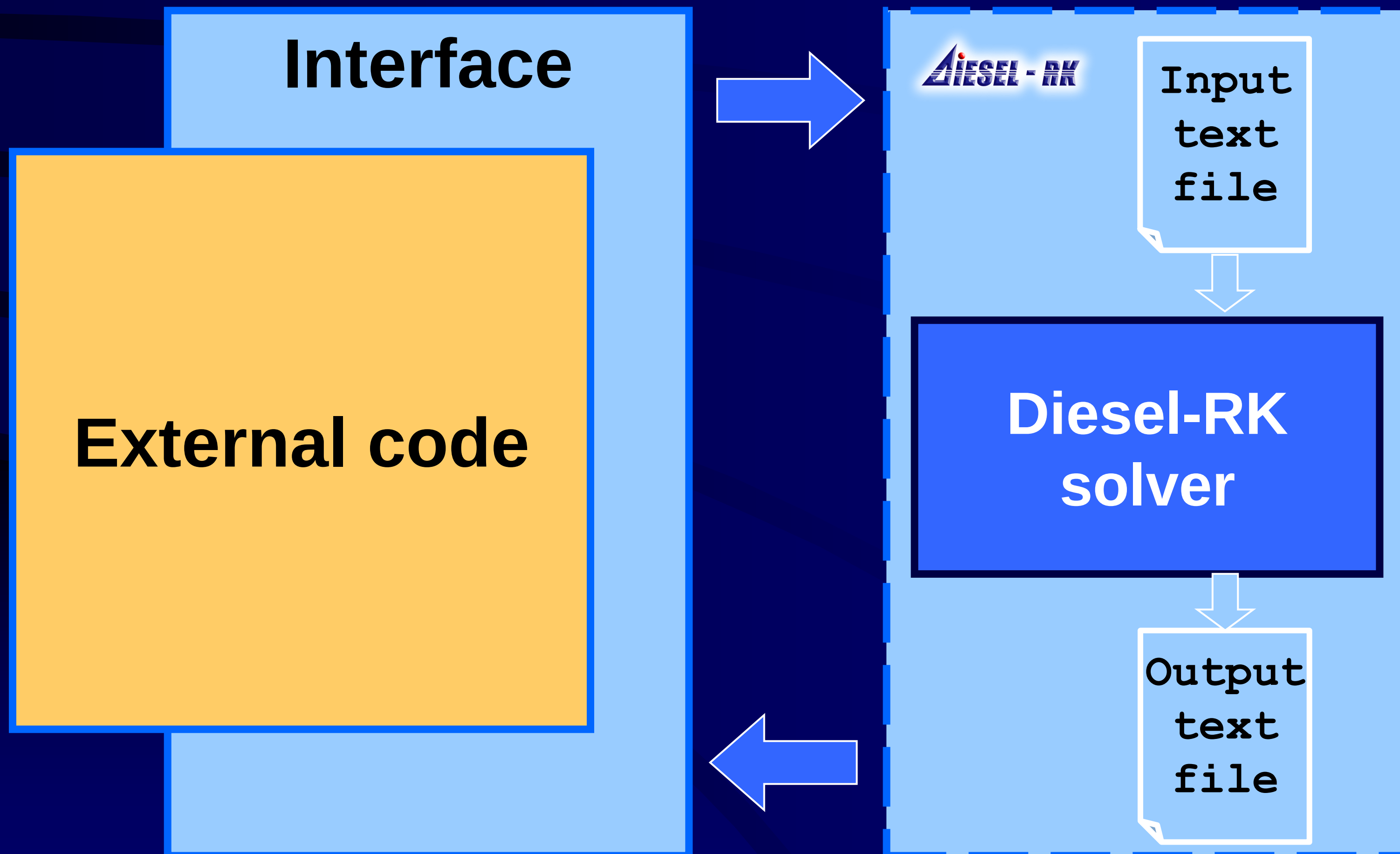
Drag & drop to assemble any combination of parts

Boundary conditions and materials properties data base

Result temperature field is used for evaporation simualtion

# Link DIESEL-RK with another Simulation Tools

Run DIESEL-RK kernel under the control of external codes



# Engine parameters optimization problem

Optimization objectives: 1. Decrease of SFC $Z_1 = SFC = f(X)$ ➡ MIN

2. Decrease of particulate matter emission (PM) and nitrogen oxides emission (NOx) together.

$$Z_2 = SE = MAX\left(1, \frac{NOx}{NOx_0}\right)^{k1} + MAX\left(1, \frac{PM}{PM_0}\right)^{k2} + \left(\frac{SFC}{SFC_0}\right)^{k3};$$ ➡ MIN

where index "0" means required values.

3. … etc.

Arguments: (independent variables)

$$\overline{X} = \left\{ \begin{array}{l} CR \\ n, dn \\ \varphi, \theta \\ PR, EGR, \text{Valve timing, Bypasses, etc.} \\ InjProf \\ PistBowl \\ \alpha, \beta \end{array} \right.$$

- CR - Compression ratio;
- n, dn - Number and Diameter of injector nozzles;
- φ, θ - Injection Duration and Injection Timing;
- PR, EGR, Valve timing, Bypasses, etc.
- InjProf - Injection profile including strategy and parameters of multiple injection;
- PistBowl - Piston bowl shape;
- α , β - Injector nozzles directions in both planes.

The structured arguments: Injection profile, Piston bowl shape, Injector nozzles design are assigned by user and may be varied by sequential retrieval.

Limits: (restrictions)

$$\overline{Y} = \left\{ \begin{array}{l} Pz \\ Pinj \\ Tt \\ SFC, \text{etc.} \end{array} \right.$$

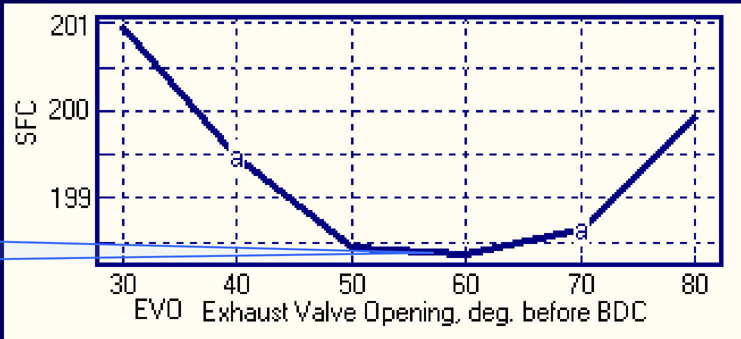
- Pz - Maximum cylinder pressure (Pz < 150 bar);
- Pinj - Maximum injection pressure (Pinj < 1500 bar);
- Tt - Temperature before turbine;
- SFC, etc.

# Solution of engine parameters optimization problem

**1D problem:** example $\begin{cases} Z_1 = SFC = f(X_1) \Rightarrow \text{MIN}; \\ X_1 = EVO \end{cases}$

Method: 1D scanning

Decision is made by user



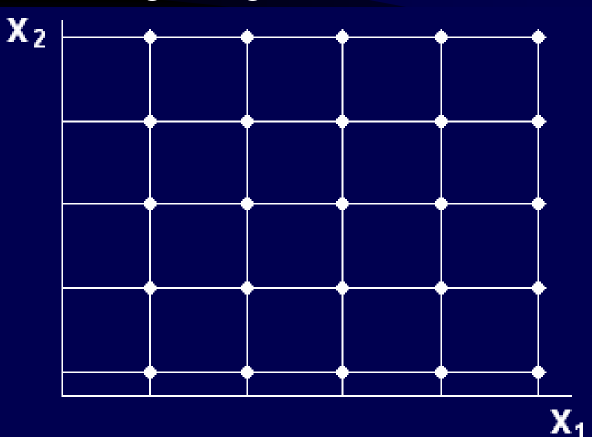

**2D problem:**

example $\begin{cases} Z_2 = SE\ (PM, NO) = f(X_1, X_2) \Rightarrow \text{MIN}; \\ X_1 = \varphi_{inj\ dur};\ X_2 = \theta_{inj\ tim};\ Y_1 = p_{inj} < 1000\ \text{bar};\dots \end{cases}$

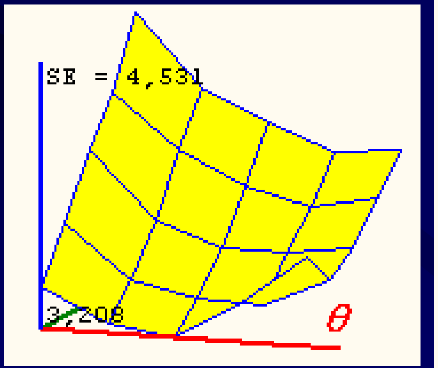
Method: 2D scanning

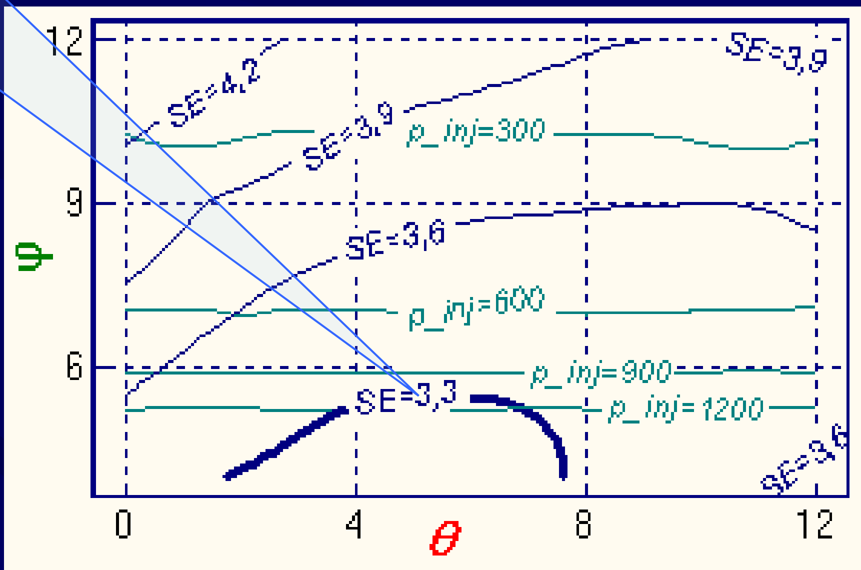
Decision is made by user

DIESEL-RK carries out the simulation of ICE in the nods of orthogonal grid.




Drag and drop technique to plot 3D diagrams and plot isolines.

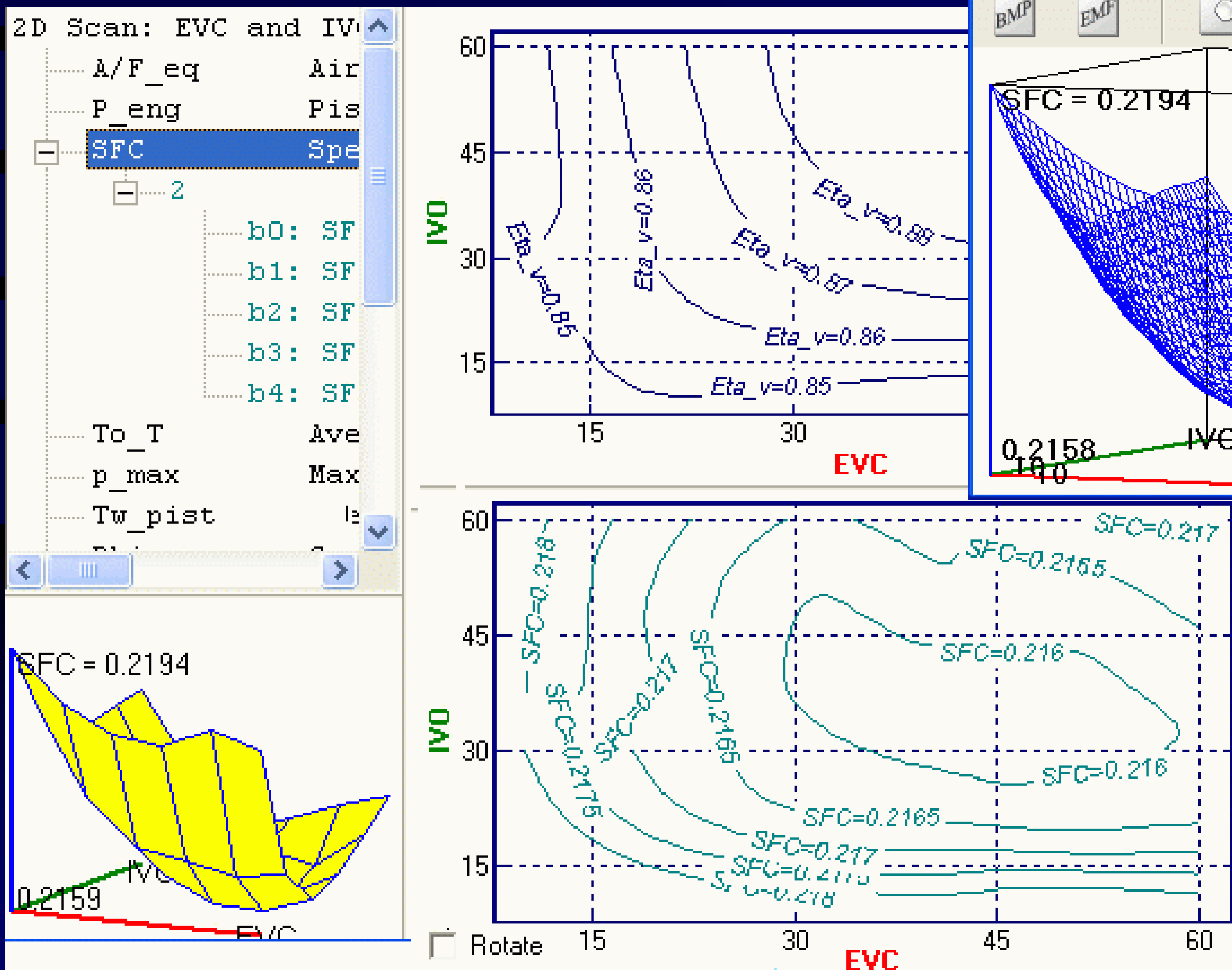


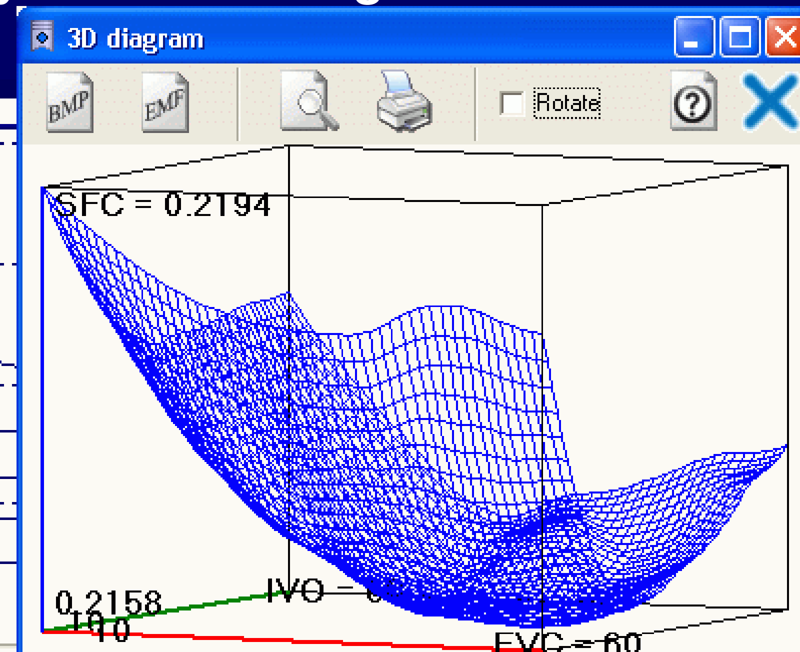




Number of nods and space are selected by user.

# 2D scanning results presentation

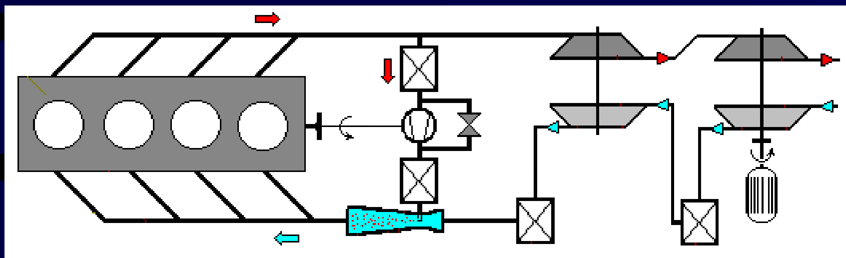
**The results of scanning may be displayed as 3-D diagram and isolines**



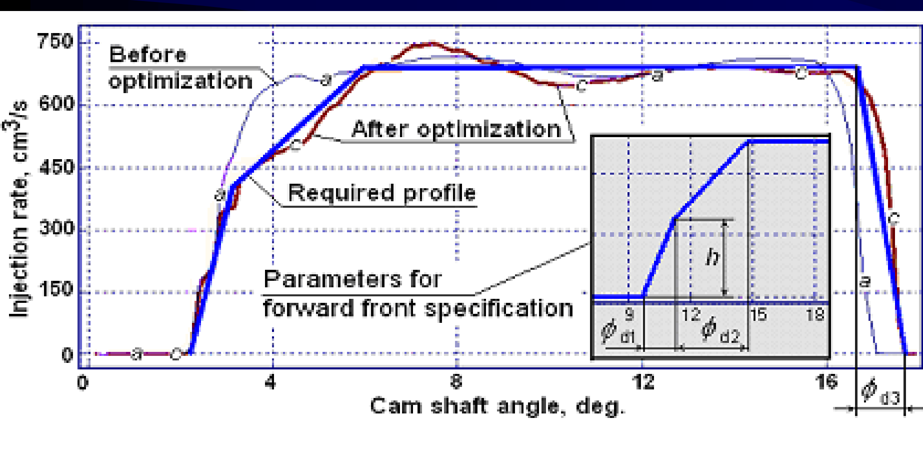
# Multidimensional optimization of engine parameters

Engine 8 parameters optimization at full load point.



8D optimization of engine parameters.

Limitations: $P_{max}$ < 200 bar.
dp/dCA < 5 bar/deg.




***Optimization results at rated power***

| Optim. particip. | Engine process param. | Values | |
|---|---|---|---|
| result | Inject. profile (fig. 10) | curve *c* | |
| parameter | IVC, deg. B BDC | 10 | 10 |
| parameter | Injector nozzle number | **10** | **9** |
| parameter | Umbrella angle α, deg. | 75 | 75 |
| independ. var. #1 | Compression ratio, CR | 14:1 | 13.5:1 |
| independ. var. #2 | Inj. nozzl. bore, $d_{inj}$, mm | 0.449 | 0.457 |
| independ. var. #3 | EGR | 0.14 | 0.121 |
| independ. var. #4 | Compressor, PR | 5.8 | 5.87 |
| independ. var. #5 | Inj. pressure, $p_{inj}$ , bar | 1596 | 1601 |
| independ. var. #6 | Inj. tim., $\Theta_{inj}$, deg BTDC | 9.2 | 10.2 |
| independ. var. #7 | Shape factor $\phi_{d2}$ | 3.0 | 4.02 |
| independ. var. #8 | Shape factor *h* | 0.6 | 0.64 |
| parameter | Shape factor $\phi_{d1}$ | 1.7 | 1.7 |
| parameter | Shape factor $\phi_{d3}$ | 1.5 | 1.5 |
| restriction | $p_{max}$, bar | 202.6 | 196.5 |
| restriction | $dp/d\phi$, bar/deg. | 4.96 | 3.82 |
| obj. func. part.#1 | NOx, g/kWh | 2.89 | 3.0 |
| obj. func. part.#2 | PM, g/kWh | 0.0184 | 0.0153 |
| obj. func. part.#3 | SFC, g/kWh | 204.2 | 205.2 |
| result | $\sigma_{liner}$, % | 0 | 1.33 |

# Solution of engine parameters optimization problem

## Multiparametrical optimization

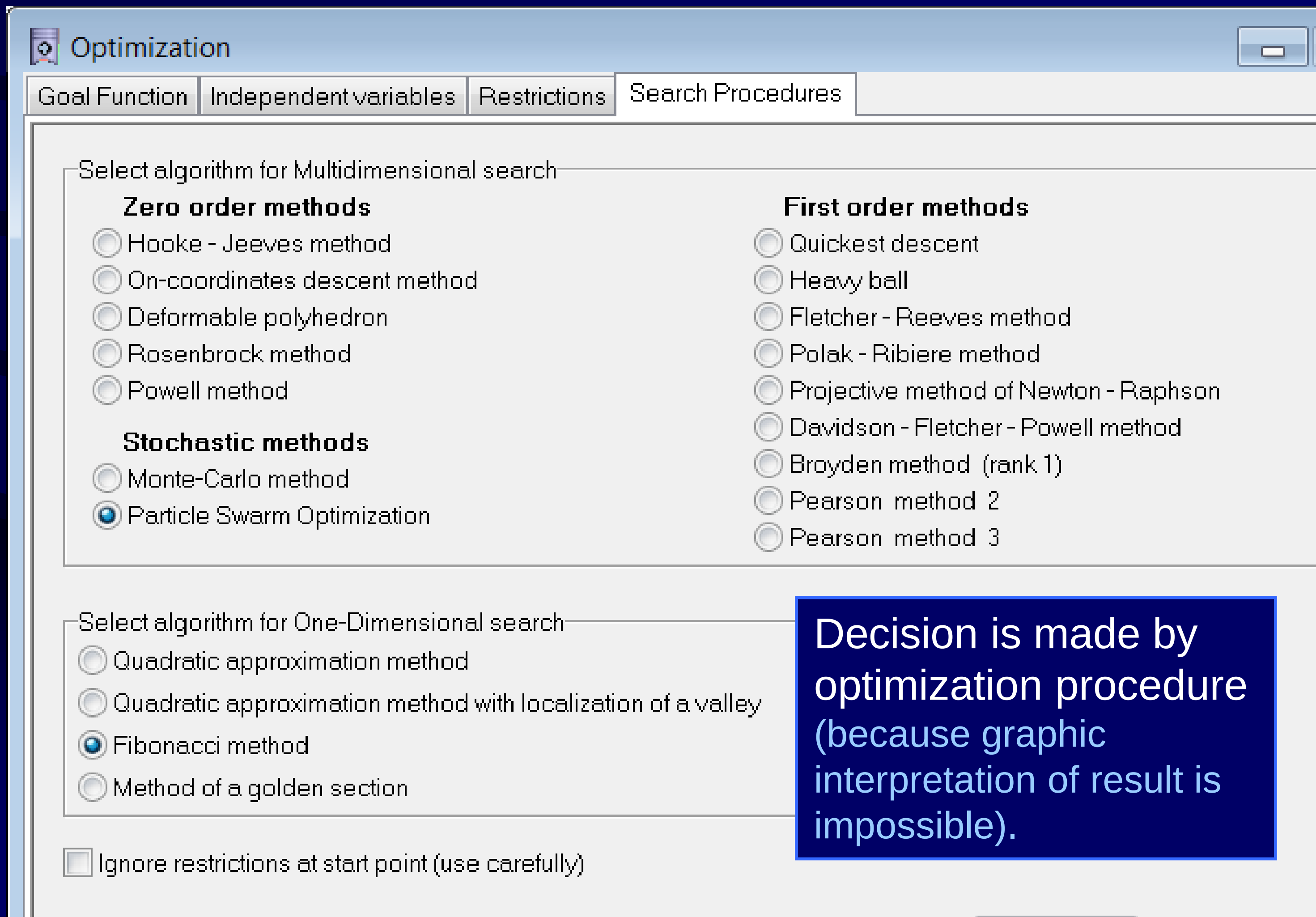
**nD problem:**

example

$$SE = MAX\left(1, \frac{NOx}{NOx_0}\right)^{k1} + MAX\left(1, \frac{PM}{PM_0}\right)^{k2} + \left(\frac{SFC}{SFC_0}\right)^{k3}; \Rightarrow \text{MIN};$$

Method:
Multiparametric optimization by means of nonlinear programming

Library of DIESEL-RK includes:
- 15 Procedures for Multidimensional optimum search and
- 4 Procedures for One-dimensional search.

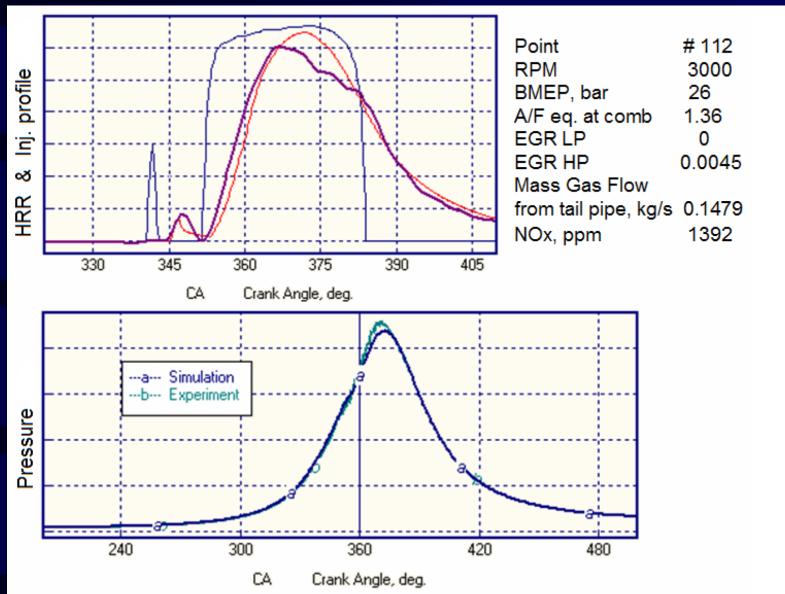


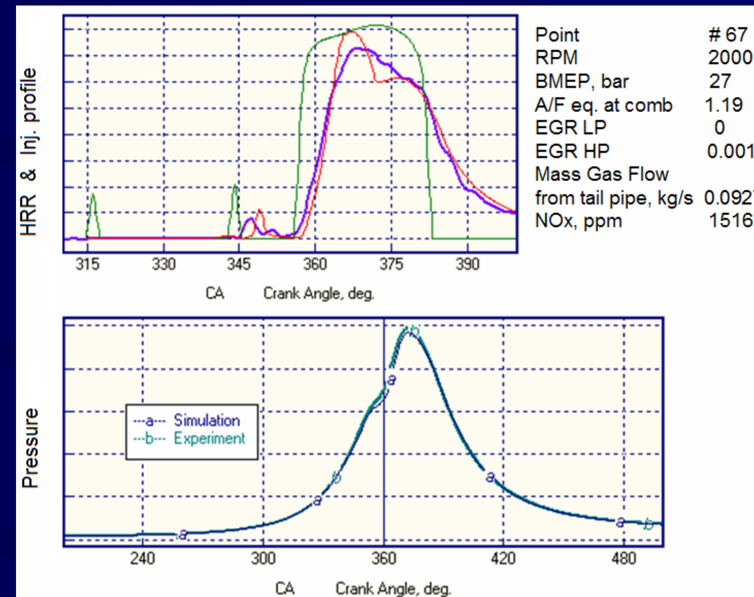

Decision is made by optimization procedure (because graphic interpretation of result is impossible).

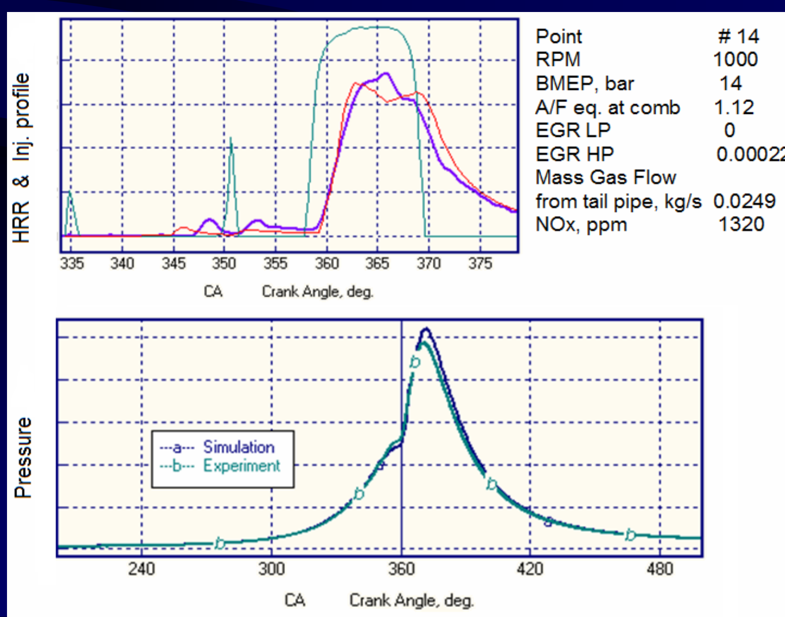
# Calibration of the combustion model of light duty diesel

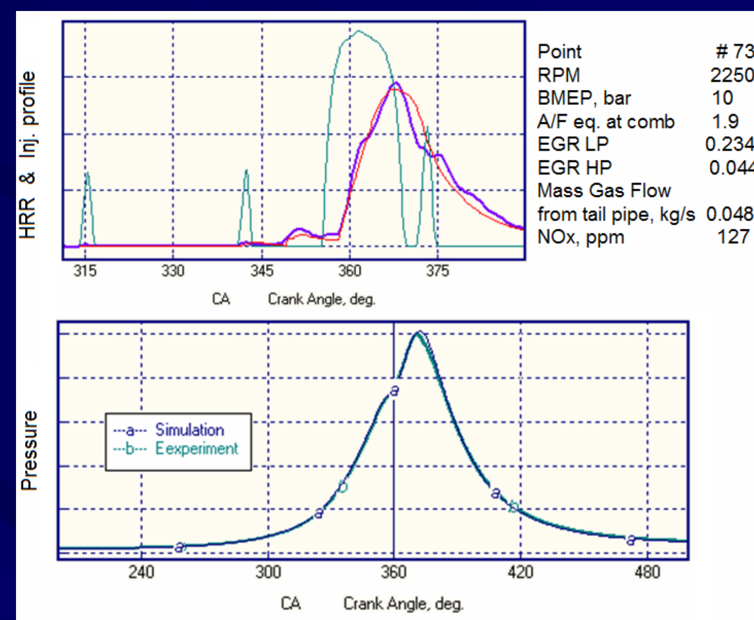
Comparison of experimental and measured HRR and in-cylinder pressure at different 10 engine operating points.

All empirical coefficients are same for each point.



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Comparison of experimental and measured HRR and in-cylinder pressure at different 10 engine operating points.

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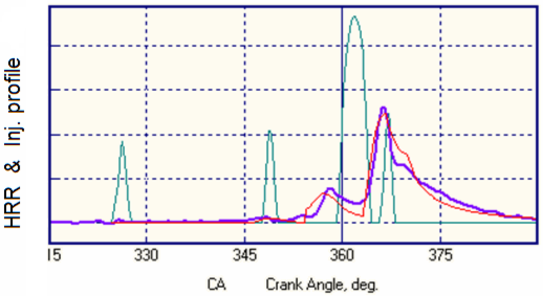
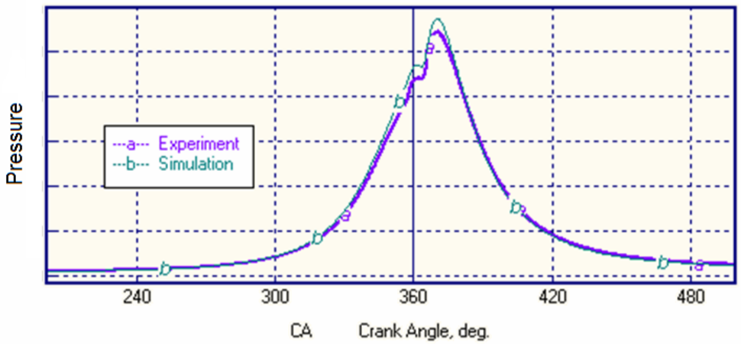
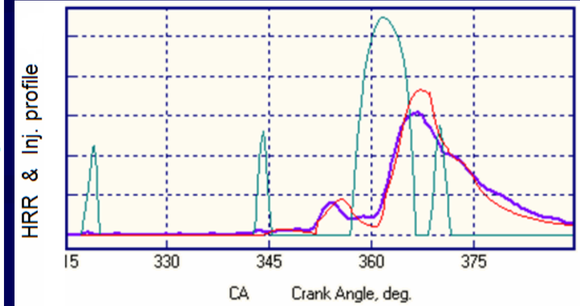
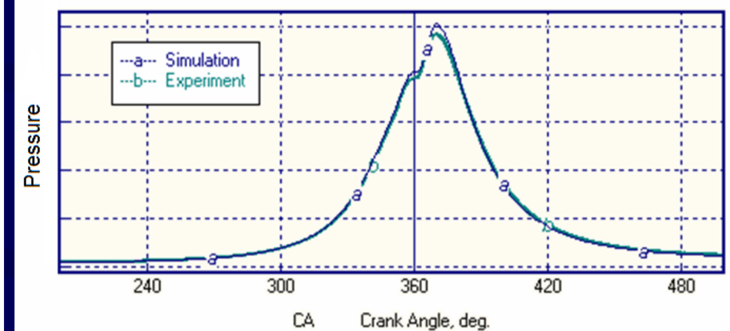


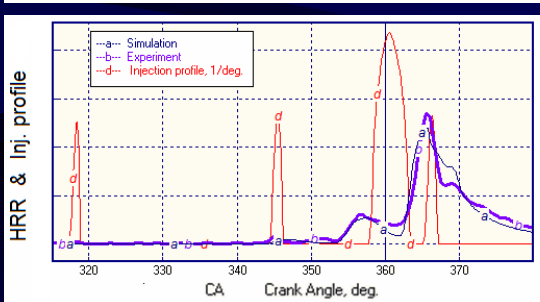

| | |
|---|---|
| Point | # 17 |
| RPM | 1250 |
| BMEP, bar | 4 |
| A/F eq. at comb | 2.54 |
| EGR LP | 0.233 |
| EGR HP | 0.1833 |
| Mass Gas Flow from tail pipe, kg/s | 0.0135 |
| NOx, ppm | 38 |



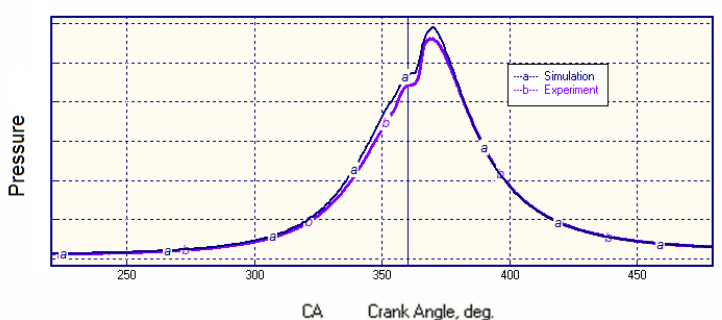



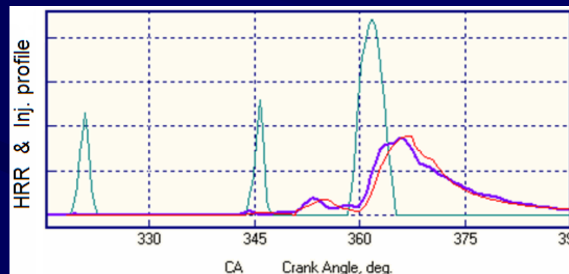

| | |
|---|---|
| Point | # 56 |
| RPM | 2000 |
| BMEP, bar | 6 |
| A/F eq. at comb | 2.4 |
| EGR LP | 0.299 |
| EGR HP | 0.044 |
| Mass Gas Flow from tail pipe, kg/s | 0.0301 |
| NOx, ppm | 76 |



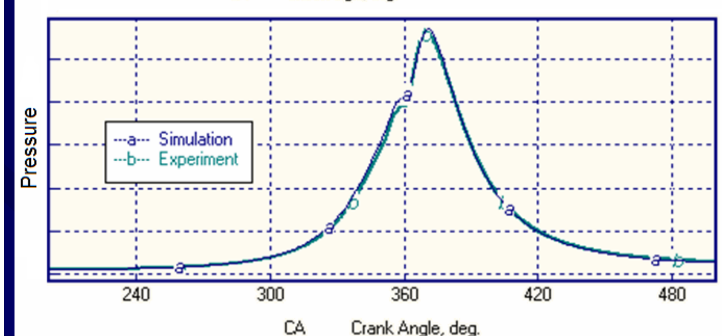




| | |
|---|---|
| Point | # 28 |
| RPM | 1500 |
| BMEP, bar | 4 |
| A/F eq. at comb. | 2.66 |
| EGR LP | 0.293 |
| EGR HP | 0.1354 |
| Mass Gas Flow from tail pipe, kg/s | 0.0163 |
| NOx, ppm | 46 |



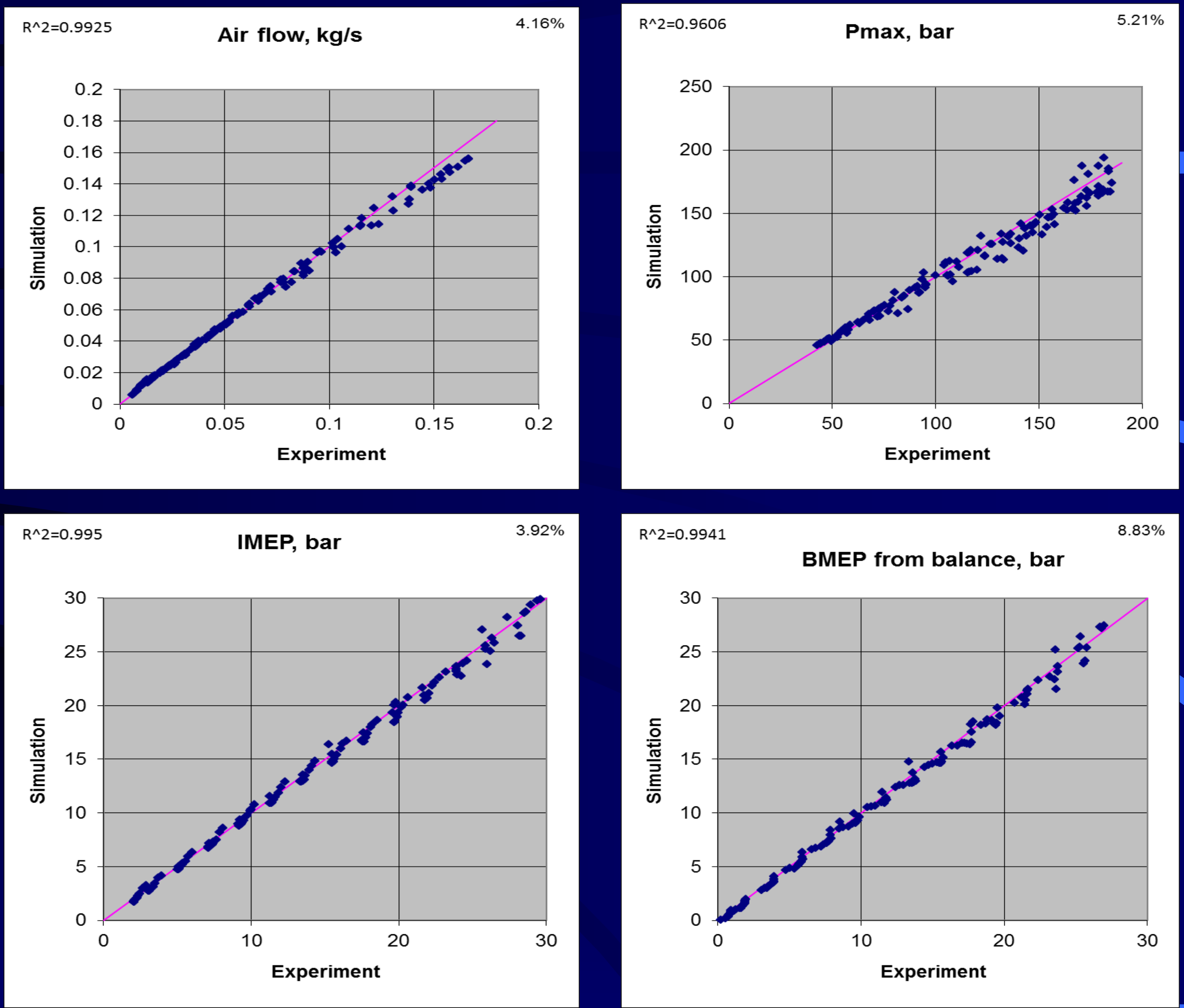

| | |
|---|---|
| Point | # 30 |
| RPM | 1500 |
| BMEP, bar | 8 |
| A/F eq. at comb. | 1.69 |
| EGR LP | 0.239 |
| EGR HP | 0.1205 |
| Mass Gas Flow from tail pipe, kg/s | 0.0237 |
| NOx, ppm | 89 |



# Calibration of the combustion model of light duty diesel

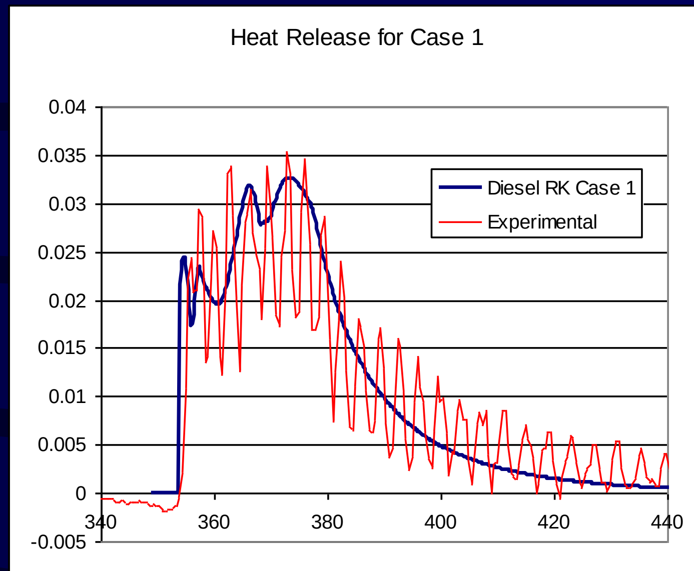
Comparison of experimental and measured engine parameters at different 137 engine operating points.

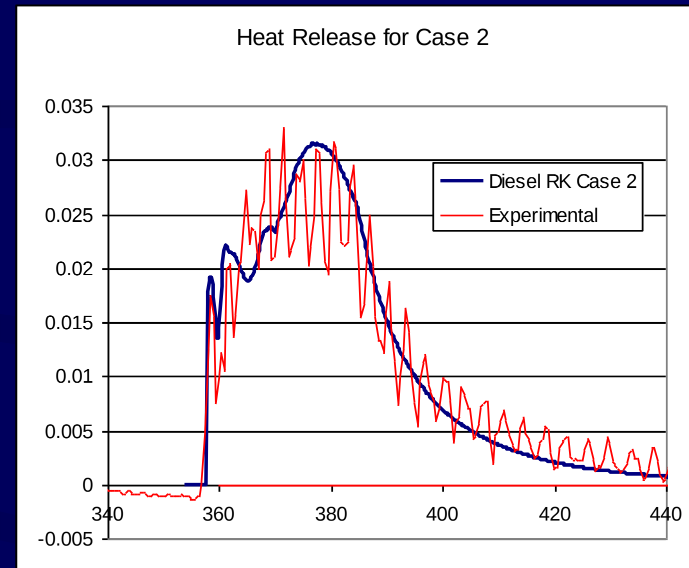
All empirical coefficients are same for each point.

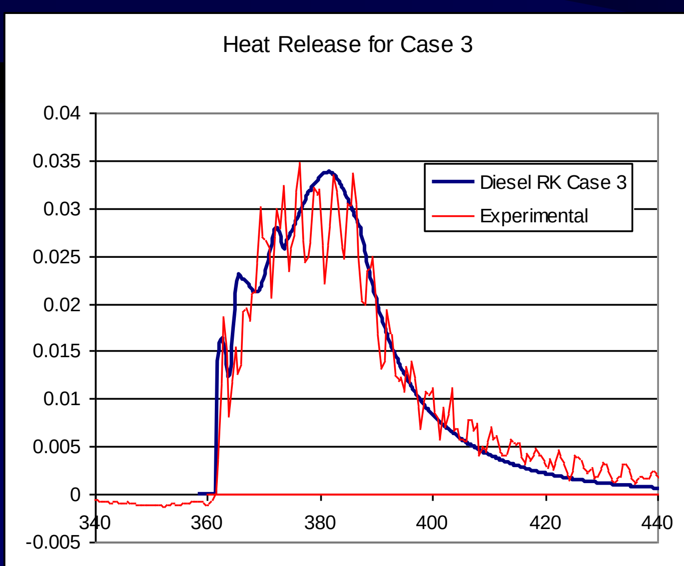


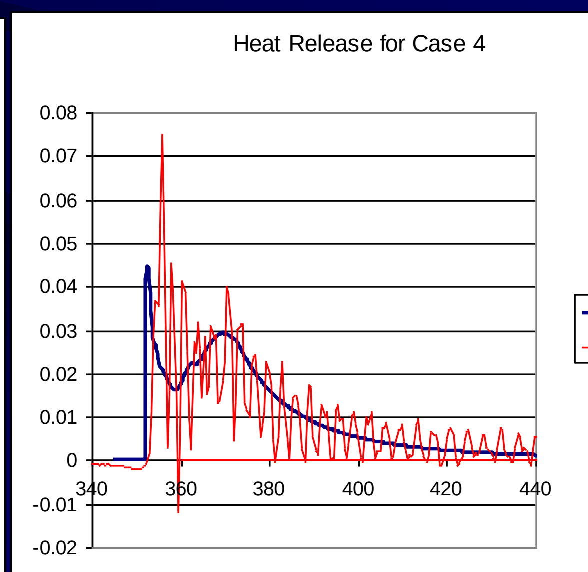
# Calibration of the model performed by GM

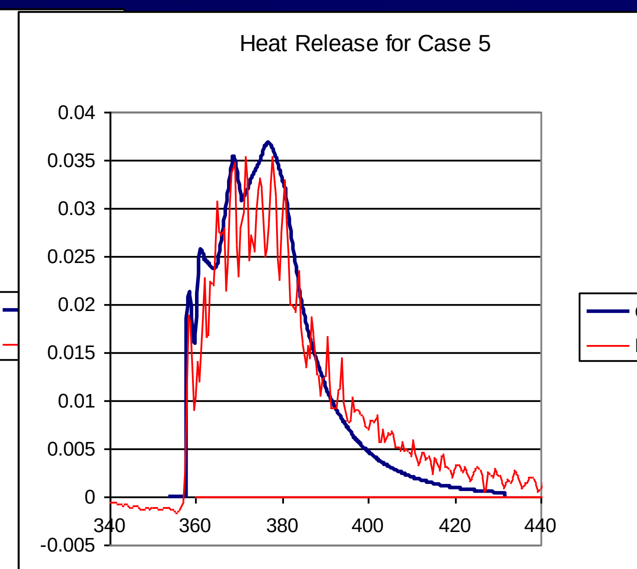
Comparison of experimental and measured parameters at different 10 engine operating points



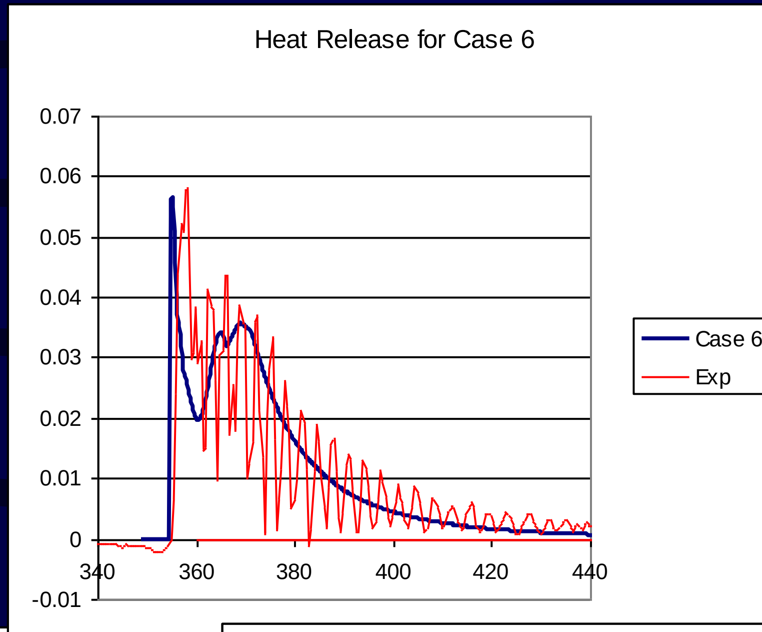



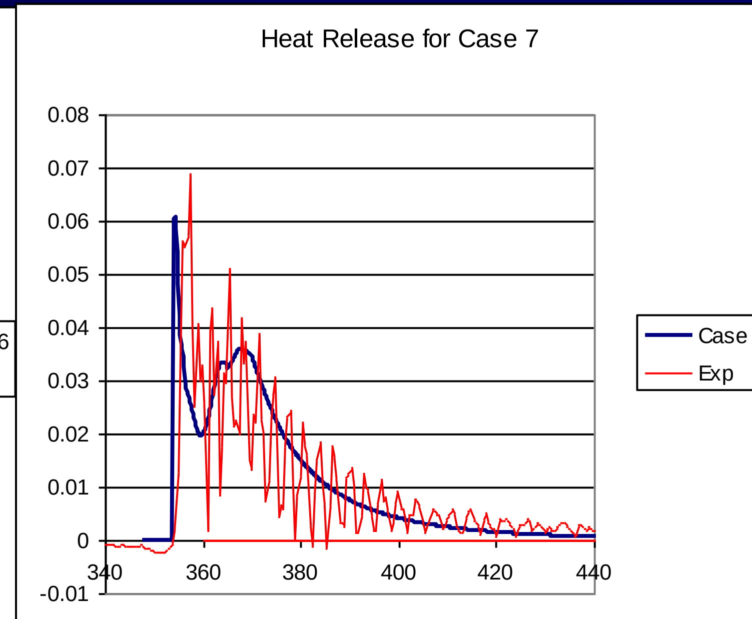



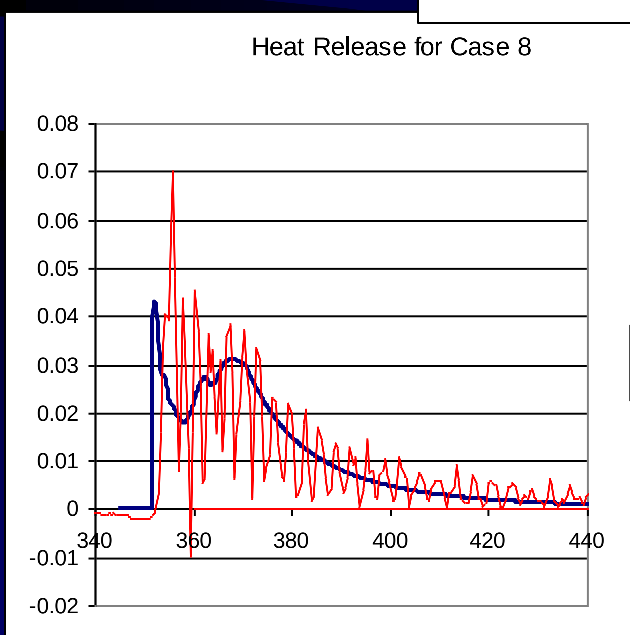



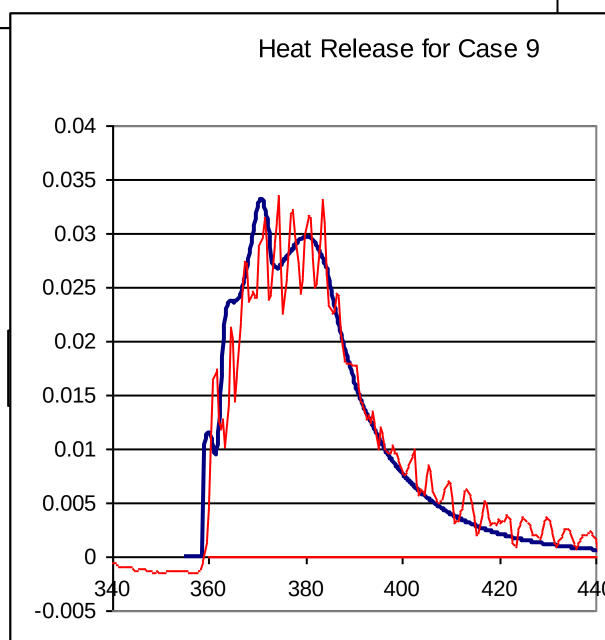
# Calibration of the model performed by GM

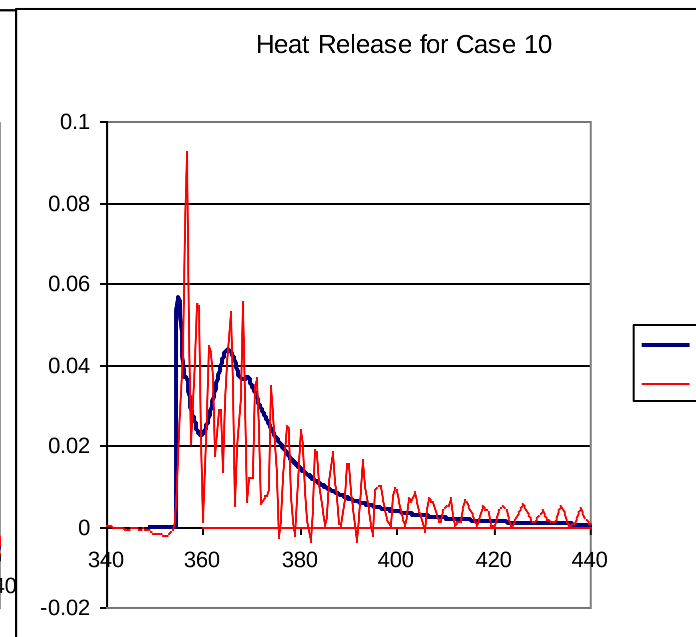
Comparison of experimental and measured parameters at different 10 engine operating points



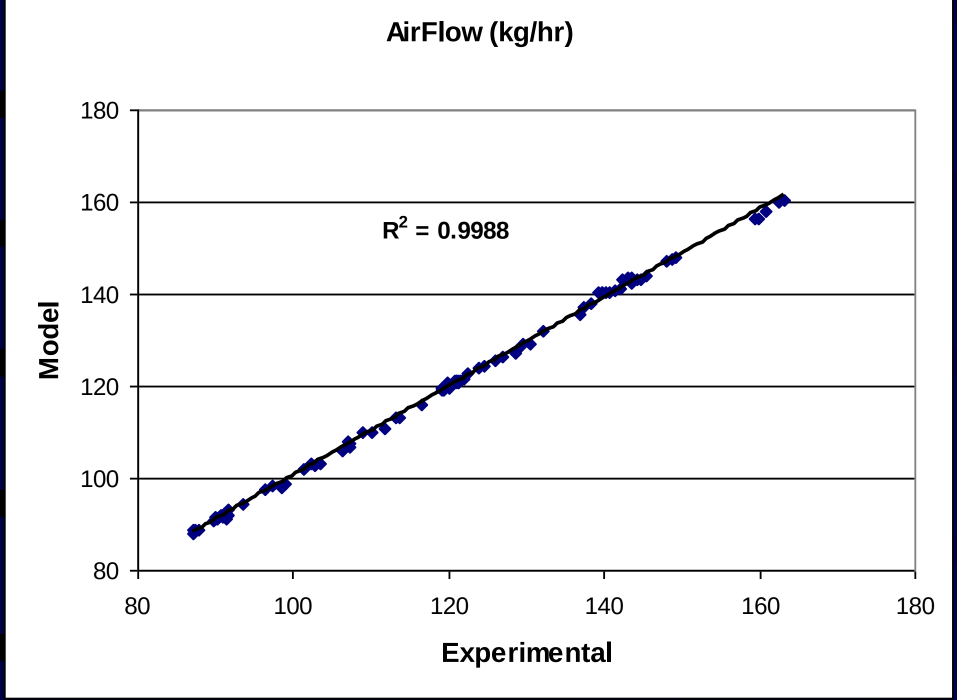



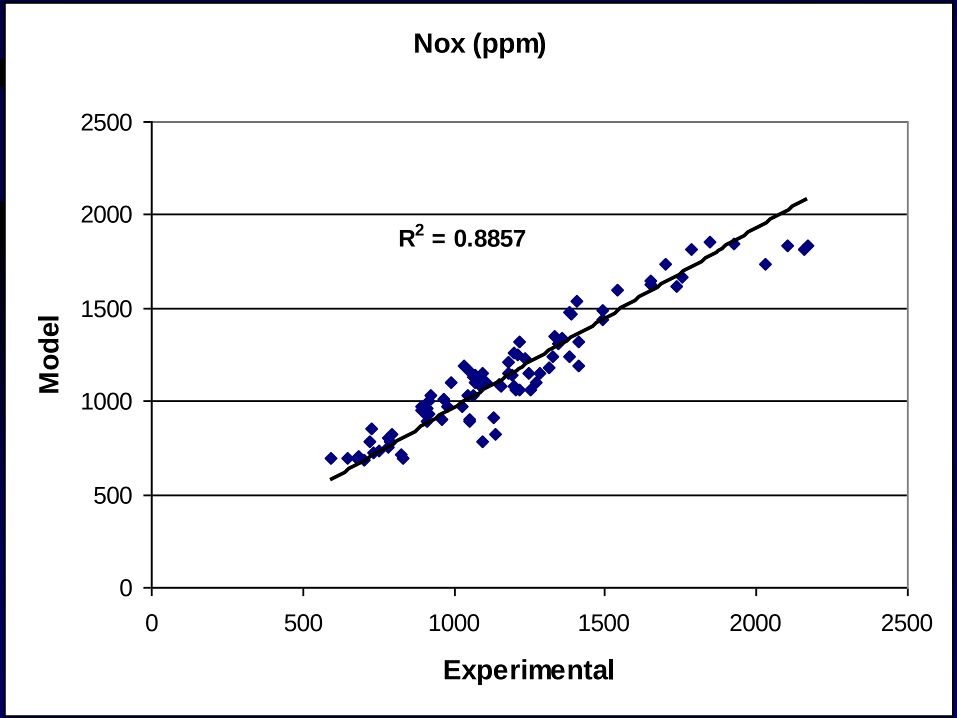
# Calibration of the model performed by GM

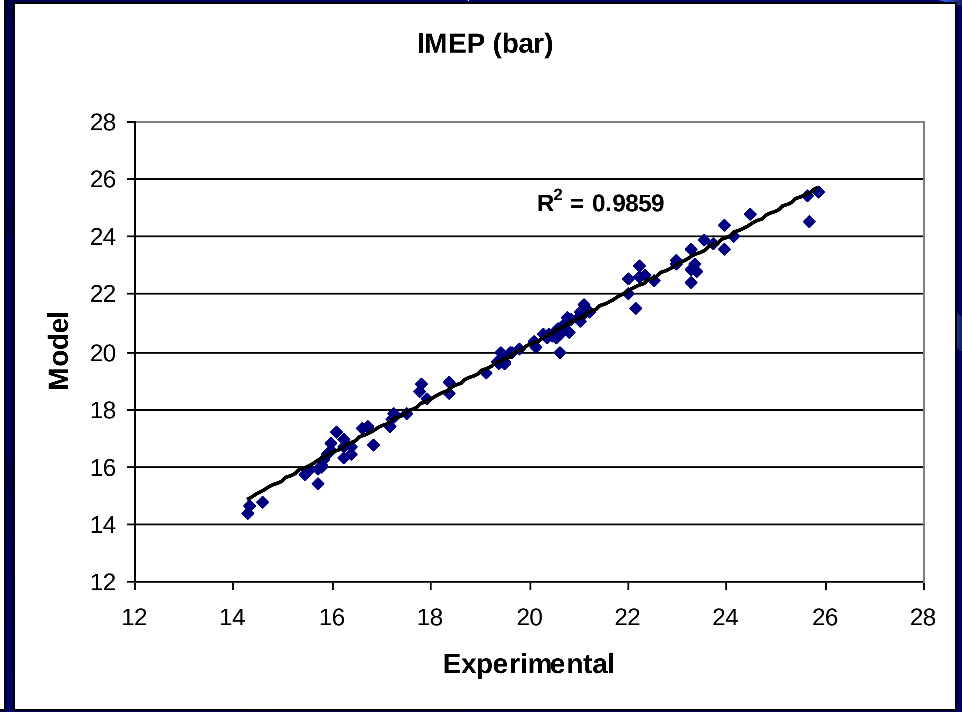



Comparison of experimental and measured parameters at different engine operating points

**89** experimental points were used

**IMEP** : Indicated mean effective pressure



# Comparison of the thermodynamic engine simulation programs

## Accessible Functions for Engine Analysis

- Difference between the cylinders
- Transient operating modes simulation
- Analysis of Noise
- List of easy diesel combustion models, including Hiroyasu model & user model.
- Link with CFD spray model using KIVA code.
- Link with valve train simulators, etc.

- Overall Engine Analysis
- Steady state operating modes
- Turbocharging analysis
- Gas Exchange analysis
- Heat Exchange analysis
- Valve Timing optimization
- 4 stroke & 2 stroke engines.
- Junkers and OPOC engines.
- Zeldovich NO formation model
- Thermodynamic EGR analysis
- Export/Import data via clipboard
- 1 parametrical researches.
- Account of the swirl at spray behavior simulation
- Phenomenological Soot model

- Express engine analysis (function of automatic engine design prediction & empiric coefficients setting for the case of data deficit)
- Gas SI engines with prechamber (arbitrary gas)
- Automatic Multi Dimensional Optimization
- 2 parametrical researches
- Advanced multi-zone DI diesel spray combustion model:
- Optimiz. of Piston Bowl Shape (& Data Base of piston bowls & advanced graphic interface)
- Optimiz. of Injector design including central & non-central sprayer as well side injection system (& 3D Fuel spray evolution visualization)
- Account of adjacent sprays interaction in volume and near the wall.
- Optimiz. of multiple injection strategy and PCCI strategy (& advanced graphic interface)
- Detail Kinetic Mechanism for NO formation (199 reactions 33 spec.)
- Bio-Fuels and blends & Data base of fuels
- Detail Chemistry (LLNL mech. 1540 reactions) at Ignition Delay simulation (PCCI / HCCI).
- Run under control of another software tools
- Coupled thermodynamic simulations with FEA (account how the local wall temperature effect in fuel evaporation)

**Existing commercial engine simulation tools**

**Specific functions**

**Common functions**

**DIESEL-RK: Specific functions**

# Additional options of DIESEL-RK

**Simulation of GAS and DUAL FUEL ENGINES.**

**- Injection of WATER;**

**- Ignition by pilot diesel injection into PRECHAMBER**