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# Multidimensional Optimization of DI Diesel Engine Process Using Multi-Zone Fuel Spray Combustion Model and Detailed Chemistry NOx Formation Model

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## ABSTRACT

A previously developed multi-zone direct-injection (DI) diesel combustion model was implemented into a turbocharged diesel engine full cycle simulation tool DIESEL-RK. The combustion model takes into account the following features of the spray dynamics:

- Detailed evolution process of fuel sprays.
- Interaction of sprays with the in-cylinder swirl and the walls of the combustion chamber.
- Evolution of a Near-Wall Flow (NWF) formed as a result of a spray-wall impingement as a function of the impingement angle and the local swirl velocity.
- Interaction of Near-Wall Flows formed by adjacent sprays.
- Effect of gas and wall temperatures on the evaporation rate in the spray and NWF zones.

In the model each fuel spray is split into a number of specific zones with different evaporation conditions. Zones, formed on the cylinder liner surface and on the cylinder head, are also taken into account. The piston bowl in the modeling process is assumed to have an arbitrary axi-symmetric shape. The combustion model supports central, non-central and side injection systems. A NOx calculation sub-model uses detailed chemistry analysis which considers 199 reactions of 33 species. The soot formation calculation sub-model used is a phenomenological one and takes into account the distribution of the droplets Sauter Mean Diameter (SMD) during the injection process. The ignition delay period is estimated using relevant data in the pre-calculated comprehensive 4-D map of ignition delays. This 4-D map is developed using CHEMKIN detailed chemistry simulations and takes into account effects of the temperature, the pressure, the Fuel/Air ratio and the Exhaust Gas Recirculation (EGR).

The noted above sub-models were integrated into full-cycle engine simulation software together with library of non-linear programming procedures, allowing multidimensional optimization of DI diesel engine working parameters to reach prescribed emissions regulations norms. List of optimized parameters includes: CR, EGR, injection profile shape, fuel injection pressure, port timings (IVC), boost pressure, power for turbocharger assistance, injection timing, nozzles hole number, diameter and inclination angle of nozzles. Two variants of piston bowl were investigated. In the research there was done an optimization of working parameters of medium speed diesel engine at few operating points with account of weighting coefficients of the points. At each operating point the problem of optimization has individual peculiarities and an individual set of independent variables and restrictions. The expression for objective function of conjoint optimization of SFC, NOx and PM was proposed. Procedures of Rosenbrock, Powell and other were used for optimum search. Restrictions were accounted by penalty function method. Controlling algorithms for EGR booster driving, injection timing, Common Rail pressure, turbocharger assist for locomotive performance were obtained. To provide a required injection profile shape being obtained in optimization a modification of injector was carried out. There were optimized fuel pipe line diameter and dimensions of internal elements of injector: control valve, orifice and internal volume. The injection profile was simulated with hydrodynamic simulation software INJECT.

## INTRODUCTION

The solutions being offered by diesel engine manufacturers to meet current and future emission regulations may be spit into in-cylinder features and exhaust aftertreatment, as shown in Figure1. The authors' research being presented in this paper deals with in-cylinder processes only. Aftertreatment in the medium speed diesels should be used only if in-cylinder technologies are insufficient.

As shown in Wartsila investigation [1] the direct water injection allows reduction of the oxides of nitrogen (NOx) emission up to 50-60%, although this technology is not used yet on engines of other manufacturers. Homogenous Charge Compression Ignition (HCCI) technology results in very low soot and NOx emissions but the issue with controlling the start of combustion almost excludes production applications of HCCI. Other technologies such as optimization of combustion, Miller cycle and exhaust recirculation are now used. Researchers and manufacturers of sate of art diesel engines publish their solutions, for example the MTU solutions [2], the MAN solutions [3]; Caterpillar solutions [4, 5]; Robert Bosch solutions [6]; Wartsila solutions [7]; AVL solutions [8]; Volvo Powertrain and Chalmers University investigation [9], etc. A summary of the above and other publications indicates the following common solutions:

- Massive cooled EGR should be up to 50%.
- Miller cycle with IVC at 10 – 15 CA deg. BBDC.
- High boost. At 25 bar BMEP 2-stage boost with total pressure ration 5.5 – 6 is required.
- Maximum cylinder pressure up to 240 bar.
- Common Rail fuel injection equipment (FIE) with maximum pressure up to 2200 bar and even up to 3000 bar (Robert Bosch) [6].
- High Air/Fuel ratio (AVL) [8].
- High Swirl (AVL) [8].
- Multiple injection (if necessary).
- Optimization of piston bowl and sprays configurations.

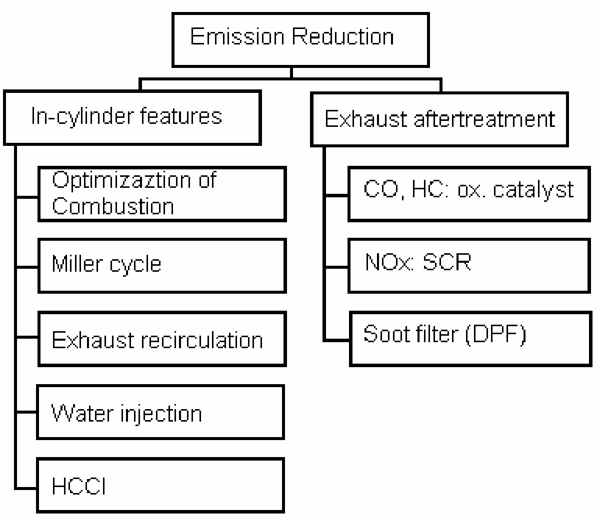


***Figure 1. Emissions reduction technologies.***

Practically, there are issues such as on one hand the selection of the most effective combination of influential control parameters, whilst on the other hand optimizing all the processes together for best fuel efficiency and reliability. Equally important what is the optimal method of using computer simulation to minimize the experimental work?

The following elements should be developed to make a computer optimization of engine parameters:

- Full cycle engine simulation software having adequate combustion and emissions models supporting the technologies shown in Figure 1.
- Fuel injection system hydrodynamic simulation software supporting non-isothermal processes and other phenomena at very high fuel pressure.
- "Mini-map" transformation of engine test cycle into corresponding steady state engine operating modes.
- Objective function specification for combined NOx, Particulate Matter (PM), Specific Fuel Consumption (SFC), etc.
- Optimization procedures.
- Concept of optimization order including selection of independent variables and constrains for every operating point. It is desirable to decrease number of optimized independent variables and use principle of physical splitting of optimization process.

These elements are described in this paper with the results of optimization obtained for a medium speed locomotive diesel engine.

## FULL CYCLE ENGINE SIMULATION SOFTWARE

A previously developed full cycle engine simulation software DIESEL-RK [10-13] was used for simulation of the engine working processes in this research. The combustion model of DIESEL-RK accounts for the following features of the spray dynamics:

- Detailed evolution process of fuel sprays.
- Interaction of sprays with in-cylinder swirl and walls of combustion chamber.
- Evolution of NWF formed after spray-wall impingement and calculated as a function of the impingement angle and the local swirl velocity.
- Interaction of NWF formed by adjacent sprays.
- Effect of gas and wall temperatures on the evaporation rate in the spray and NWF zones.

In the model each fuel spray is split into a number of specific zones (Figure 2) with different evaporation conditions.

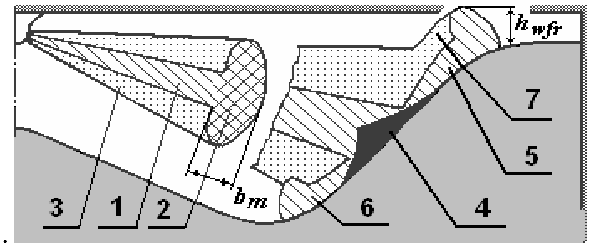


***Figure 2. Characteristic zones of the diesel spray.***

Prior to the jet impingement, only the following three zones are considered in the spray:

1. Dense conical core.
2. Dense forward front.
3. Dilute outer sleeve.

The NWF which is formed by the spray's impingement is inhomogeneous in structure, in density and in temperature, which makes the calculation of fuel evaporation very difficult. It is therefore convenient to split the NWF into several zones with averaged heat and mass transfer coefficients. This is done by analogy with the free spray division into typical zones. After the impingement, new zones are considered as follows:

4. Axial conical core of the NWF.
5. Dense core of the NWF on the piston bowl surface.
6. Dense forward front of the NWF.
7. Dilute outer zone of the NWF.

Zones, formed on the cylinder liner surface and on the cylinder head, are also taken into account. The piston bowl in the modeling process is assumed to have an arbitrary axi-symmetric shape. The combustion model supports central, non-central and side injection systems.

To make possible an optimization of multiple injection strategy (including the PCCI concept) the combustion model supports Low Temperature Combustion [12] and prediction of self ignition delay by means of detail chemistry simulation [13]. The pre-calculated comprehensive 4-D map of ignition delays is used. This 4-D map is developed using CHEMKIN detailed chemistry simulations and takes into account effects of temperature, pressure, Fuel/Air ratio and EGR on the ignition delay period.

The phenomenological soot formation/oxidation sub-model takes into account distribution of the droplet SMD during injection process and peculiarities of heat release.

DIESEL-RK supports the use of Venturi nozzle to mix exhaust gas taken before turbine with air after the charge air cooler if the boost pressure slightly exceeds the inlet turbine pressure.

In the previous researches the models of DIESEL-RK have been validated using published and provided by manufacturers experimental data obtained on high-, medium- and low speed engines. Comparison of results demonstrates a good agreement between theoretical and experimental sets of data. Mainly these researches were done under contracts with engine manufacturers and part of them is published in references of table 1. The comparison of calculated and measured data for locomotive performance of medium speed engine D49 being a similar to the engine investigated here is presented in Appendix A. Because experimental data is not available for the engine studied in this paper the calibrations of D49 were used for it.



The engine scheme being used in current research is presented in Figure 3 in which 1 is EGR pump, 2 is the Venturi nozzle, 3 and 4 are the intercoolers, 5 is a motor for turbocharger assistance, 6 are EGR coolers. The investigated medium speed diesel has a Stroke/bore diameter=310/265 mm; and a BMEP=26 bar @ 1000 RPM. The engine has tandem intake and exhaust ports so a slight swirl is presented in the cylinder. In this research the effect of the swirl was accounted but one was not investigated (optimized).

***Table 1. References on results of validation of diesel simulation software with experimental data***

| 4 stroke diesel engines | Applic. | D/S, mm | Source |
|---|---|---|---|
| Peugeot DW10-ATED4 | Car | 85 / 88 | [12,13,16] |
| ZMZ 514 | Car | 87 / 94 | [11] |
| KamAZ 7405 | Truck | 120 / 120 | [11,12,15] |
| YaMZ 238 | Truck | 130 / 140 | [11] |
| CAT 3401 | Research | 137 / 165 | [14, 16] |
| M756 | Locom. | 180 / 200 | [16] |
| D49 | Locom. | 260 / 260 | [11, 16] |
| D42 | Marine | 300 / 380 | [16] |
| D50 | Locom. | 312 / 330 | [16] |
| 2 stroke diesel engines | | | |
| D100 (opposite piston) | Locom. | 207 / 2 x 254 | [16] |
| Mitsubishi UEC45LA | Marine | 450 / 1350 | [15] |
| B&W 74 VT2BT - 160 | Marine | 740 / 1600 | [16] |

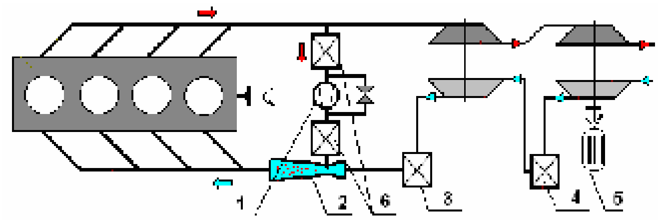


***Figure 3. Engine scheme.***

## CALCULATION OF NOX FORMATION USING THE DETAILED KINETIC MECHANISM

To account for possible massive EGR the NOx calculation sub-model uses detailed chemistry analysis which considers 199 reactions of 33 species [10]. Combustion of complex hydrocarbons occurs by stages: 1 - the first stage is very fast disintegration of a fuel molecule on radicals and molecules with smaller number of atoms; 2 - further there is considerably slower process of delayed burning in which particles with one - two atoms of carbon participate.

For simplification of the description of the first stage of combustion for more complex, than methane, hydrocarbons (components of diesel fuel, biofuel, DME) the gross-reactions which describe disintegration of the higher hydrocarbons and their derivatives up to simple molecules and radicals are entered. Initial disintegration kinetic of a fuel molecule is described by 40 reactions with participation of 10 species. It is supposed, that regardless of initial composition of hydrocarbon at its combustion in the second phase participate the same simple hydrocarbons. Therefore for the description of delayed burning process the non-empirical detail kinetic mechanism of combustion of the elementary hydrocarbon – methane is used. The kinetic scheme of NO formation at combustion of the methane is compiled on the basis of the kinetic scheme by prof. Basevich V.J. [17]:

$CH4 + O2$ Û $CH3 + HO2$
$CH3 + O$ Û $H + H2CO$
. . . . . . . . . . . . . . . . . .
$CH + N2$ Û $HCN + N$
$N + O2$ Û $NO + O$.

The given scheme consists of 199 reactions and determines concentration of 33 species: CH4, C2H, C2H2, C2H3, C2H3O2, C2H4, C2H5, C2H6, CH, CH2, CH3, CH3O, CH2O, CHO, CO, CO2, H, H2, H2O, H2O2, HO2, O, O2, OH, N2, N, NO, NO2, N2O, HNO, NH, HCN, CN.

The scheme includes reactions being responsible for both thermal and prompt nitrogen oxides. The material balance of the species participating in chemical reactions is described by system of the kinetic equations (1):

$$\left.\begin{array}{l}
\dfrac{dC_1}{d\tau} = \pm k_1 C_j C_k \pm k_2 C_l C_m \,\mathrm{K}\, \pm k_{199} C_p C_r\,; \\
\dfrac{dC_2}{d\tau} = \pm k_1 C_a C_b \pm k_2 C_c C_d \,\mathrm{K}\, \pm k_{199} C_e C_f\,; \\
\mathrm{K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K\,K} \\
\dfrac{dC_{33}}{d\tau} = \pm k_1 C_\alpha C_\beta \pm k_2 C_\gamma C_\delta \,\mathrm{K}\, \pm k_{199} C_\varepsilon C_\zeta\,.
\end{array}\right\} \qquad (1)$$

where: $C_j$, $C_k$ ,… $C_\zeta$ are mole fraction of the appropriate substances; $\tau$ is time; $k_i$ are the constant of chemical reaction rate, determined on Arrhenius equation:

$$k_i = A \times T^n \times exp(-\frac{E}{R \times T}) \qquad (2)$$

where: A is pre-exponential factor, $n$ is an exponent, $E$ is energy of activation, $R$ is absolute gas constant. The numerical solution of the differential equations system (1) is carried out by Gear's method with variable order of accuracy.

## FUEL INJECTION SYSTEM SIMULATION SOFTWARE

A previously developed fuel injection system hydrodynamic simulation software INJECT [18] was used for engine fuel system design and optimization. To enable analysis of systems with pressure greater than ca 2500 bar INJECT accounts for non-isothermal processes due to compression and heat transfer. The tool supports two-phases gas-fluid state of fuel, hydraulic resistance in unsteady flows, sound velocity variability, volumetric or mass balance in volumes, flexibility (elasticity) of a fuel-injection pump drive and multi-mass torsional system behavior of the pump drive, and simulation of transient operation of the fuel systems. Any fuel system may be designed for analysis with INJECT which uses large elements for project creation. Figure 4 presents the Common Rail system of the medium speed diesel engine.

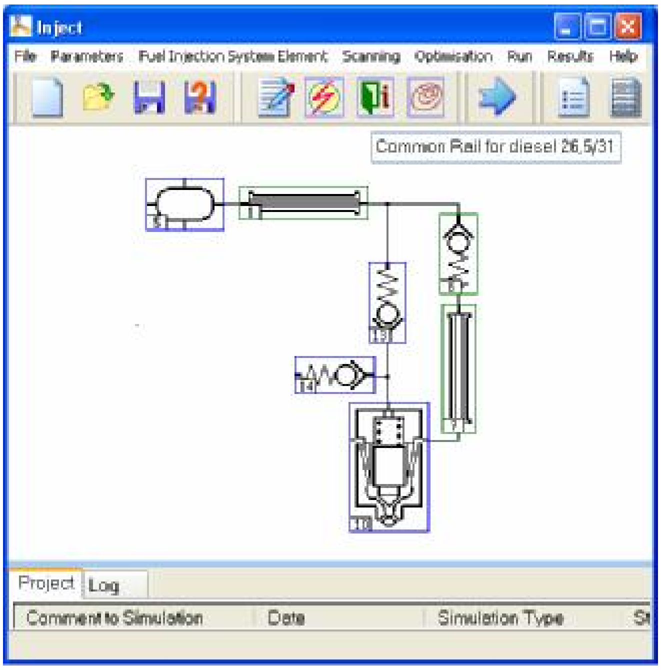


***Figure 4. Engine CR fuel injection system simulation scheme.***

The friendly GUI allows modification of FIE parts and simulation of the whole system behavior at any operating mode, comparing the resultant curves to the target values.

## OBJECTIVE FUNCTION FOR OPTIMIZATION

The optimization target generally includes minimization of SFC within emissions constraints and practical limits such as maximum combustion pressure, maximum rate of cylinder pressure rise and the fuel rail pressure.

Selection of the engine operating points for optimization depends on specific test cycle. If the engine simulation tool does not support transient engine operation and focused on the steady state modes the specific test cycle should be transformed into the engine mini-map steady-state test points with corresponded weighting coefficients as it shown in the Figure 5. This transformation is done with account of vehicle

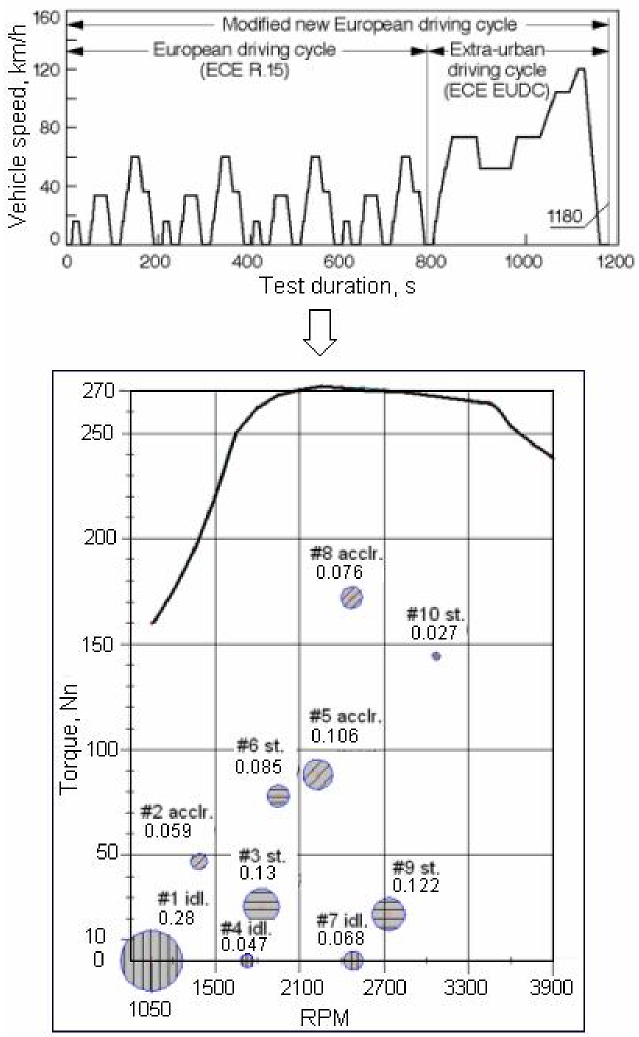


***Figure 5. Vehicle driving cycle and corresponding engine operating map with weighting coefficients***

mass and powertrain characteristics. The area of every engine operating point in the performance map corresponds with the weighting coefficient $C_i$ being used for the total emissions calculation, as in equations (3).

$$NOx_{sum} = \frac{\sum_{i=1}^{n} C_i\, NOx_i}{\sum_{i=1}^{n} C_i\, P_i}, \qquad PM_{sum} = \frac{\sum_{i=1}^{n} C_i\, PM_i}{\sum_{i=1}^{n} C_i\, P_i}; \qquad (3)$$

where: $NOx_i$ and $PM_i$ are emissions in g/hour at the *i*-operating point; $P_i$ is engine power in kW at the *i*-operating point; *n* is a number of operating points in optimization research (in the Figure 5, *n*=10).

For the locomotive engine studied here, the operating map with weighting coefficients of every operating point is presented in the Figure 6. Here: $n = 3$; $C_1 = 0.6$, $C_2 = 0.25$, $C_3 = 0.15$. The weighting coefficients here are defined by standard.

A contribution of every operating point to total emissions is different, as illustrated by Figure 7, obtained for the engine with high boost provided by 2-stage free turbocharger. The full load operating point is critical for NOx emissions and half of the maximum BMEP operating point is critical for the PM emissions. This means the high injection pressure should be provided for on the full load point and the 35% load point. Only a Common Rail system can keep high fuel pressure at part load. .

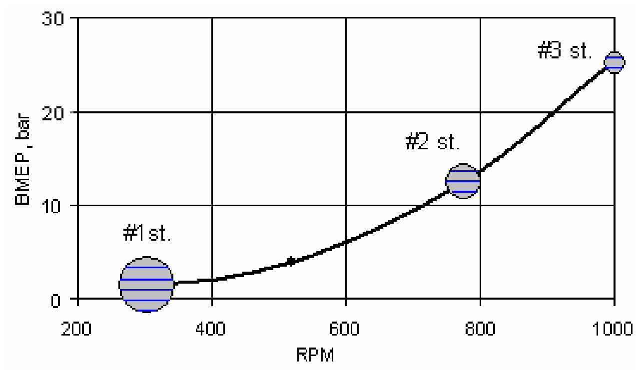


***Figure 6. Locomotive engine operating map with weighting coefficients***

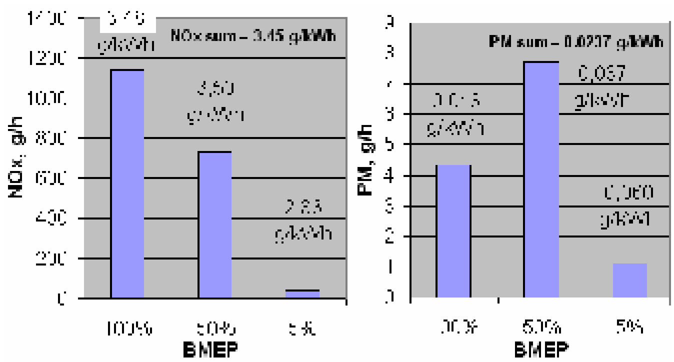


***Figure 7. Contribution of operating points to total emissions of locomotive engine with free running turbocharger***

A Pareto optimization may be used to find an optimum combination of several affecting factors in case of several simultaneous objective functions such as SFC, NOx and PM. These optimization tools are known and presented on the market [19]. The multi-target optimization algorithm is successfully used in previous researches but here we used another and more economical way of one target optimization which does not require so large number of engine simulation sessions. Algorithms of one target optimization are developed well and they are very economical. There are few published researches focused on transformation of multi-target optimization into one target optimization, for example Montgomery and Reitz [20] proposed following expression:

$$SE = \frac{1000}{\left(\frac{NOx+HC}{(NOx+HC)_0}\right)^2 + \left(\frac{PM}{PM_0}\right)^2 + \left(\frac{SFC}{SFC_0}\right)}; \quad (4)$$

Desantes et al. [21] proposed expression:

$$SE = \left(\frac{SFC}{SFC_0}\right) + \exp\left[k_1\left(\frac{NOx - NOx_0}{NOx_0}\right)\right] + \exp\left[k_2\left(\frac{PM - PM_0}{PM_0}\right)\right]; \quad (5)$$

where: $SFC_0 = 210$, $NOx_0 = 3.5$, $PM_0 = 0.02$, are fuel consumption and emissions in target region; $k_1$ and $k_2$ are coefficients to vary the pollutants decrease. Equations (4) and (5) allow Total Emissions (SE) to be decreased even in the zone where: $NOx < NOx_0$ and $PM < PM_0$ , although it is not required and associated with increased fuel consumption. To improve the optimum search in this research another expression is proposed:

$$SE = MAX\left(1, \frac{NOx}{NOx_0}\right)^{k1} + MAX\left(1, \frac{PM}{PM_0}\right)^{k2} + \left(\frac{SFC}{SFC_0}\right)^{k3}; \quad (6)$$

where: $k_1$=2.0, $k_2$ =2.0 and $k_3$ =2.0 are coefficients to vary the pollutants and SFC decrease. Working with expression (6) a search procedure tries to improve other constituents only if one of them has achieved a target value. An alternative is to use SFC as a objective function and NOx & PM as constrains. However, this is analogous to use of equation (6), if penalty function method is used.

## PROCEDURES FOR OPTIMUM SEARCH

Because a task of optimum search may include at least 6 or more independent variables, a search procedure should have 0 or 1 order, i.e. procedure may use or not use only the first derivatives of target function. Non-linear programming does not indicate in advance what search method is preferable, so the software being developed for optimization problems and being used in this paper includes a library of 14 optimization methods including random search (Monte Carlo method). The use of these 14 methods is not unnecessarily superfluous because the theory may not guarantee what kind of optimum is found, e.g. local or global. One way to check the optimum is to perform additional searches from the same start point but with other search procedures, and then compare results. More over the Monte Carlo method allows searching for an optimum located “over a hill” and use of intermediate points as a starting points for a search with other formal procedures.

## CONCEPT OF OPTIMIZATION ORDER

During the optimum search it is desirable to decrease a number of dimensions of the optimization problem and use a principle of physical splitting of investigated processes. For example, it is possible to separate a combustion intensity control and an arrangement of the injected fuel allocation to prevent a cylinder liner wetting and oil dilution. The latter is important at full load operating modes where there is a lack of available space for the spray plumes and for NWF radial penetration. On the other hand it is possible to select separately the parameters of Miller cycle: Intake Valve Closing (IVC) and additional boost pressure to compensate losses of fresh charge. Optimum point of Miller cycle may be placed “over a hill” and formal procedure of optimum search may not be able to find it. First step of optimization is a setup of initial approach. In this paper the initial approaches were taken from diesel D49, from published data noted above and from preliminary simulations.

### Optimization of Miller cycle parameters

Selection of the timing for Intake Valve Closing (IVC) is one of the local optimization task which may be resolved separately by means of 2D scanning. The procedure of 2D scanning includes simulation of engine operation in the junctions of the 2D grid having relatively large steps in both dimensions, as shown in Figure 8. Beyond the coarse grid is transformed into fine grid by a Delaunay triangulation method; a linear, or spline interpolation may also be used. Finally the iso-contours are plotted to find an optimal point, as per Figure 8.

Early close of the intake valves should be compensated by additional boost, so in the 2D scanning a compressor Pressure Ratio (PR) and IVC were varied to arrange the rough grid of engine parameters variations. The results in Figure 9 show a constant value of PM emission along the green line with an Air/Fuel equivalence of 1.84. Simultaneously, NOx emissions and combustion pressure decrease with earlier IVC. The optimum IVC of 10º BBDC is selected as compromise of acceptable Air/Fuel ratio and minimum boost pressure, as suggested in published research for NOx<3.5 g/kWh and PM < 0.025 g/kWh. The Compressor PR obtained here is used at the next steps of optimization as initial approach or a start value.

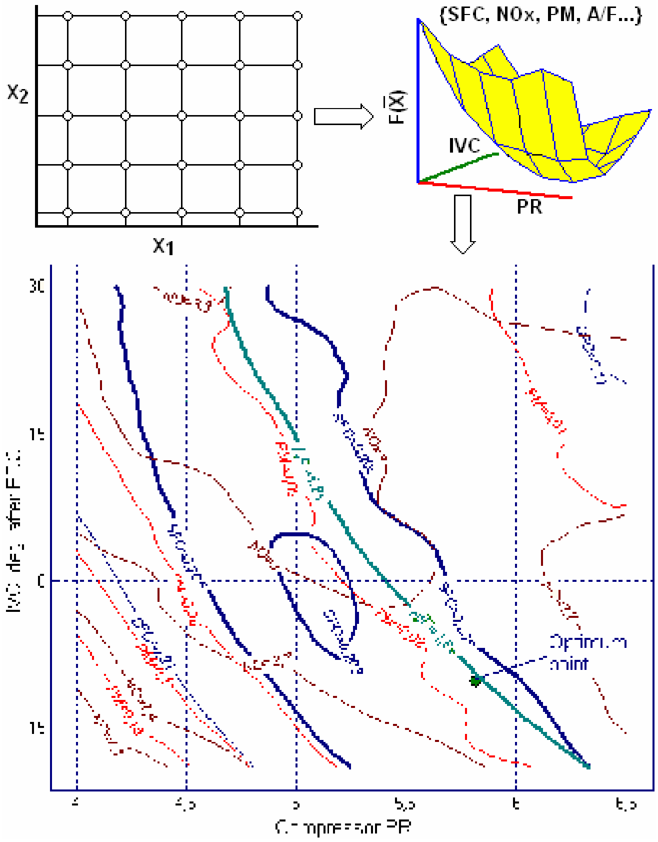


*Figure 8. Effect of Compressor Pressure Ratio and Intake Valve Closing (Miller cycle) on the locomotive engine parameters at full load*

## Selection of piston bowl and optimization of nozzle inclination angle

Two concepts of piston bowls were investigated, Figure 9. CR is controlled by above piston clearance *hp*.

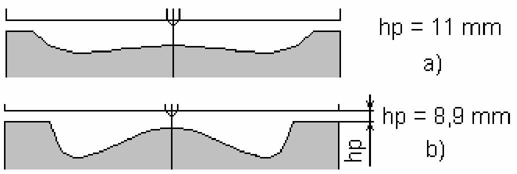


*Figure 9. Variants of piston bowl: a – shallow; b – medium.*

For both bowls and for 3 variants of nozzles having 8, 9 and 10 holes there were carried out 2D parametrical researches where diameter of nozzles and injection timing were varied at constant value of injection pressure $p_{inj}$ = 1600 bar. Variation of nozzles diameter at $p_{inj}$ = const. allows account automatic variation of injection duration and spray tip (and NWF) penetration. Total number of 2D parametrical researches was 6, two of them having best fuel efficiency are presented in Figure 17, Appendix B. The target of this research is detection of preferable piston bowl and first approach of number and diameter of nozzle holes. Both 9 and 10 holes nozzles have shown about same fuel efficiency and NOx emission at varying the holes diameter from 0.45 up to 0.5 mm, Figure 17, Appendix B. The average value of diameter: 0.47 mm was selected for parametrical research being focused on accurate definition of umbrella angle α for every piston bowl. Figure 10 represents an effect of α on distribution of injected fuel and soot emission for the case of shallow piston bowl. Here σ means fractions of fuel allocated in the characteristic zones of fuel spray.

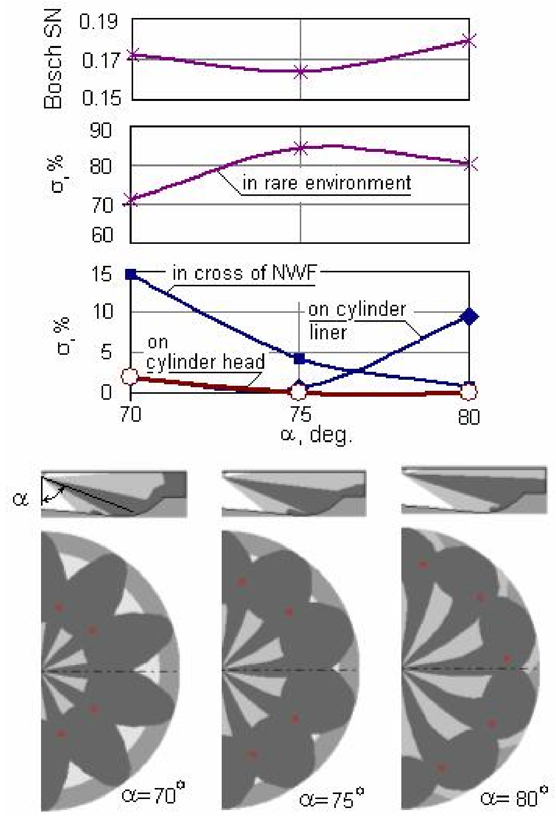


*Figure 10. Effect of umbrella angle on distribution of injected fuel and soot emission of locomotive engine with shallow piston bowl*

At the small α (=70$^0$) the free spray penetration is shorter, the impingement angle is acute and the near wall flow evolves mainly in the radial direction with about 4% of fuel reaching the liner, half of this fuel reaching the cylinder head surface. Due to the relatively cool temperature of these surfaces the evaporation rate here is smaller. On the other hand, at α=70$^0$ the fuel fraction of the dilute zones of free spray and NWF becomes smaller due to the more intensive crossing of NFW of adjacent sprays: there is 15% of the fuel located in the crossing zones. More intensive crossing of NFW takes place due to the sprays impingement point approaching the bowl center. Soot emission grows due to both phenomena. At $\alpha = 80^0$, the free spray reaches the cylinder liner directly and $s_{liner}$ = 9.5%. This is unacceptable if cylinder liner does not have a fire ring as the temperature of this zone will be relatively low, evaporation becoming slow and combustion efficiency decreasing. As well it is dangerous due to possible lubrication oil dilution by diesel fuel. So, the optimal solution of this local task is a spray umbrella angle of $\alpha = 75^0$.

The results of analogous parametrical research but for the case with medium piston bowl are presented in the Figure 11.

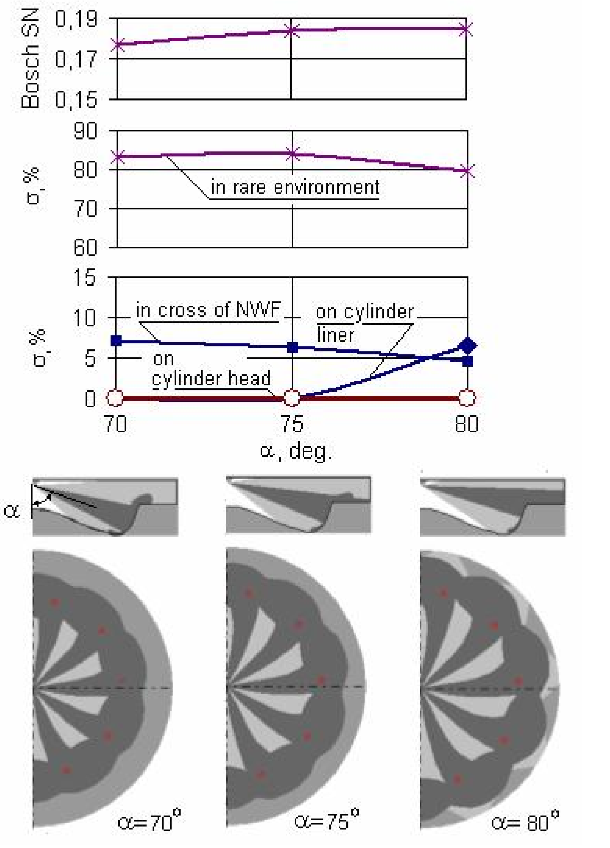


***Figure 11. Effect of umbrella angle on distribution of injected fuel and soot emission of locomotive engine with medium piston bowl***

The obtained results demonstrate the medium piston bowl is not so sensitive to umbrella angle as the shallow bowl. But soot emission in the case of medium bowl is larger than minimum value provided by shallow bowl at $\alpha = 75^0$. The larger soot emission takes place due to peculiarities of NWF evolution in the deep piston bowl: angle of spray and wall impingement here is near to $90^0$, and NWF penetrates in all directions. So a fraction of fuel in zone of crossing NWF is larger and the use of air in above piston clearance is smaller. A deep piston bowl is preferable in medium speed engines where density of compressed air in the cylinder is insufficient to brake fuel spray and prevent a wetting of cylinder liner. The shallow piston bowl is a best for engine having BMEP > 22 bar. Shallow bowl has smaller area of heat exchange and allows allocation of more fuel in volume of dilute outer surrounding of spray. This zone has best conditions of evaporation. The tool being used here allows investigate any piston bowl shape, so this step of the research may be expanded on any number of different variants of piston bowls if it will be necessary.

## 8D optimization of engine parameters at rated power

The next step of combustion optimization is to search for combinations of following parameters at rated power:

1. Compression ratio (CR) in the cylinder.
2. EGR ratio. If boost pressure exceeds the turbine inlet pressure such that the Venturi nozzle is insufficient to mix exhaust gas with air, the power of EGR pump is calculated and accounted in the engine power balance.
3. Compressor Pressure Ratio (PR). The turbine inlet pressure is calculated from the power balance of turbine and compressor.
4. Injector nozzles diameter ($d_{inj}$). The injection duration is calculated automatically as a function of injector nozzles effective flow area and fuel injection pressure.
5. Injection pressure (before nozzles) ($p_{inj}$). Due to technological and cost limitations the injection pressure was varied up to only 1600 bar. It was assumed the Common Rail pressure is limited to 1800 bar.
6. Injection timing ($Q_{inj}$).
7. Shape of injection profile.

The following limitations were used for the optimum search. The maximum cylinder pressure was set to 200 bar, and the maximum cylinder pressure rise limited to 5 bar/crank degree.

An IVC = $10^0$ BBDC was fixed to keep Miller cycle concept. The number of nozzles was varied from 8 up to 11 as parameter (it means optimum search sessions where carried out independently for every hole number). The shallow piston bowl was used only because one was selected as optimal in the previous step. A shape of injection profile was specified parametrically using shape factors $f_{d1}$, $h$, $f_{d2}$ and $f_{d3}$, (Figure 12) described below. These factors being included into list of independent variables of optimization together with injection pressure and nozzles diameter allow specify injection profile for every engine simulation during optimum search. After every optimization session termination the obtained injection profile (parametrical) was reached by hydrodynamic simulation. The design of FIE was varied to achieve a good agreement of obtained in optimization parametrical injection profile with real profile provided by system with account of wave and dynamic effects. In other words, the FIE was modified to provide required performance (plotted by blue bold line in the Figure 12) as close as possible. The essences of these modifications together with scheme of FIE are described in the Appendix C. There is general trend to make both rise of the injection rate at the very beginning and decrease of injection rate at the end of injection as rapid as possible. So these parameters ($f_{d1}$ and $f_{d3}$) may be excluded from optimization process and assigned corresponding with hydrodynamic simulation results obtained in previous iteration. The sequence of optimization is presented in Figure 13.

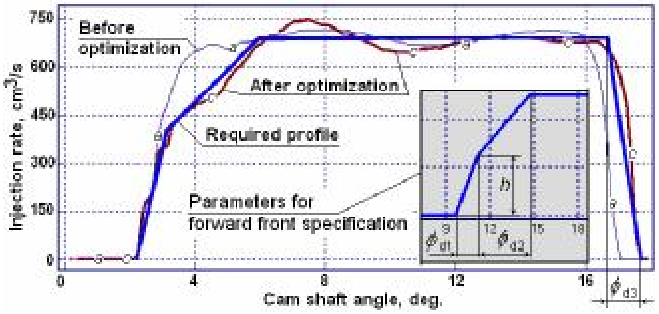


*Figure 12. Injection profiles being obtained at optimization at full load operating mode*

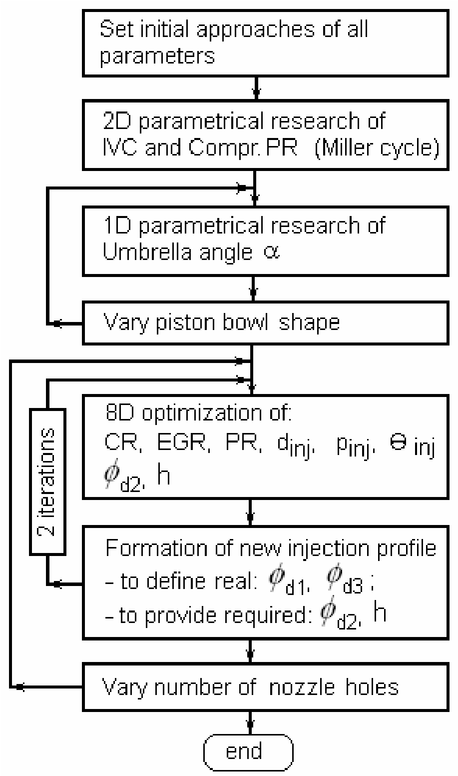


*Figure 13. Order of engine parameters optimization at full load operating mode*

The optimization was carried out by several methods from same starting point. There were used methods of Rosenbrock, Powell, Nelder-Mead and coordinate descent method. All methods lead to similar results; it allows making a conclusion about the correctness of the obtained solution. The Rosenbrock method was the most efficient. Finding a solution in one optimization search the using the Rosenbrock method required 90 – 110 sessions of engine simulation (20 – 25 minutes of computer time (PC Dualcore 2GHz)). For comparison: the Powell's method requires in 1.5 more simulation sessions to find optimum. The results being obtained for 9 holes nozzle and for 10 holes nozzles are presented in the Table 2.

The fast leading rate of injection (straight up to maximum, curve *a* in Figure 12) providing small soot emission may not be optimal when there is a limit of in-cylinder pressure rise rate. In this case, the optimum is a profile with two areas of fuel flow increase. The duration of the flow rise of every area is controlled by the following shape factors. $f_{d1}$ is a duration of fuel flow rapid rise at the beginning of injection [in CA deg.]; $f_{d2}$ is a duration of moderate flow rise at the second part [in CA deg.]; *h* is a relative height of inflexion point where fuel flow rise becomes smaller, as shown by the grey zone in Figure 12. The deployment of such new fuel injection profile still limits the duration of the injection process part in which there is a low pressure and large SMD of droplets being a source of soot emission. But at the same time such new profile limits the pressure rise rate $dp/df$ in the cylinder.

*Table 2. 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., $Q_{inj}$, deg BTDC | 9.2 | 10.2 |
| independ. var. #7 | Shape factor $f_{d2}$ | 3.0 | 4.02 |
| independ. var. #8 | Shape factor *h* | 0.6 | 0.64 |
| parameter | Shape factor $f_{d1}$ | 1.7 | 1.7 |
| parameter | Shape factor $f_{d3}$ | 1.5 | 1.5 |
| restriction | $p_{max}$, bar | 202.6 | 196.5 |
| restriction | $dp/df$, 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 |

The optimal leading rate of the injection profile obtained in this work is shown in Figure 12 versus the required profile (blue bold line). The bold red line *c* shows the real injection profile being obtained at the last iteration.

Both solutions for 9 and 10 holes show about same results but solution with 10 holes looks preferable because one has not fuel fraction allocated on the cylinder liner ($\sigma_{liner} = 0$).

## Optimization of engine parameters at part load points

One outcome of the previous work was an acceptable injection profile and FIE design. This injector and all FIE were used for all further steps of the investigation. After the boost pressure was derived at rated power point, the turbine and compressor maps were taken from a prototype and scaled for the engine of this work.

The number of optimized parameters at the 50% BMEP point may be decreased to:

1. Injection timing.
2. EGR ratio.
3. Boost pressure. In the case of an electrically / hydraulically assisted turbocharger, a corresponding power may be used as argument of optimization; for turbocharging control, a control parameter may be included into the optimal search. In all cases, turbine and compressor maps are used to define the compressor and turbine parameters. In the case of a free turbocharger, the boost pressure is defined from matching maps and one is excluded from the list of optimized parameters.

The first optimization variable (the injection timing) is the control parameter of the Common Rail system. A second control parameter is fuel pressure in the accumulator; a pressure level was accepted $p_{inj}$ = 1600 bar (as at full load), based on practical recommendations. So, the injection profile was calculated only once before the optimization and this profile was used at the optimum search. A 3D optimization was done and the results are shown in the Table 3.

***Table 3. Results of optimization at the part load***

| Optim. particip. | Engine parameter | Value | Value |
|---|---|---|---|
| | Rated BMEP | *50%* | *5%* |
| independ. var. #1 | $Q_{inj}$, deg BTDC | 9.0 | 1 |
| independ. var. #2 | EGR | 0.16 | 0 |
| result | Compres. PR | 3.0 | 1,05 |
| independ. var. #3 | Power for TC assistance, kW | 13 | 0 |
| parameter | $p_{inj}$ , bar | 1600 | 450 |
| obj. func. part.#1 | NOx, g/kWh | 3.26 | 3.53 |
| obj. func. part.#2 | PM, g/kWh | 0.0226 | 0.047 |
| obj. func. part.#3 | SFC, g/kWh | 202.3 | 310 |

Optimization of engine parameters at the 5% BMEP operating point is not required, because a contribution of this mode into total emissions is small and the modes with 100% and 50% BMEP have provided some safety margin. Neither EGR nor assistance for turbocharger are required for the light load point. The simulation results of engine parameters are presented in Table 3. The contributions of every operating point to the total emissions is presented in Figure 14. Comparison of Figure 7 and Figure 14 shows a large advantage for assisted turbocharging to the total emissions of NOx and PM. This is mainly due to the boost pressure margin at 50% load, allowing increased Air/Fuel ratio, decreased soot emissions, increased power perfecting performance as well.

The optimization of the other operating points using the same technique enables the derivation of algorithms for the control of EGR, FIE and turbocharger assistance. The fuel rail pressure ($p_{rail}$) and start of injection (SOI) as well as the % EGR and power of EGR pump drive (Power EGR pump) are presented in the Figure 15 versus engine speed. The EGR pump drive uses less than 1% of engine power at every operating mode. Turbocharger assistance is used at part load points only, and at the investigated operating points the turbocharger power assistance is less than 3% of the engine power. It is probable that at engine speeds less than 600 RPM, the TC assistance power would be a large if required engine capacity has to be increased. The predicted engine performance and emissions are presented in Figure 15.

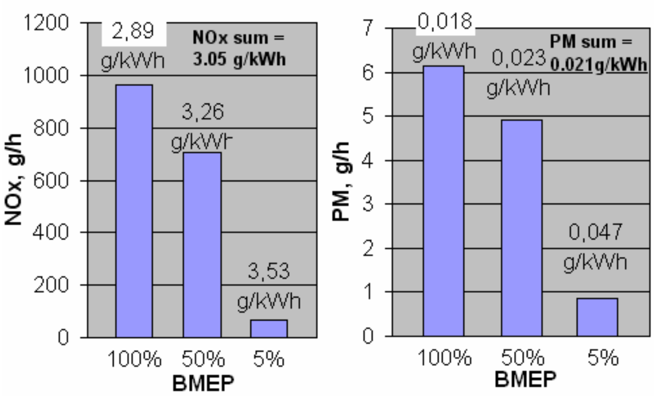


***Figure 14. Contribution of operating points into total emission of locomotive engine with assisted turbocharger***

The total emissions calculated by equations (3) with account of weight coefficients are NOx = 3.052 g/kWh and PM = 0.021 g/kWh.

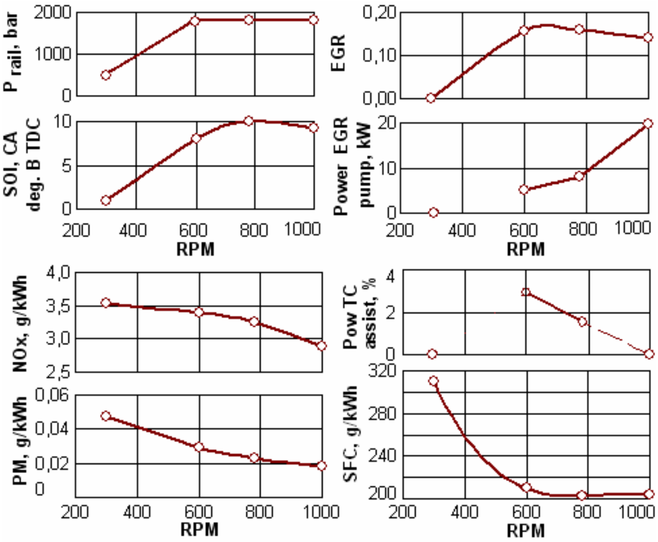


***Figure 15. Engine locomotive performance and characteristics of fuel injection system control, TC assist control and EGR system control***

# SUMMARY/CONCLUSIONS

A procedure is proposed for engine parameter predictive optimization using a combination of engine simulation, fuel system simulation and nonlinear optimization procedures. The technology finds solutions to meet prospective emissions regulations for a prescribed engine. This procedure is based on the following considerations and aspects.

- Generalized solutions to meet modern emissions regulations for medium speed engines are known and published, but this computerized procedure enables identification of specific engine control parameters. A multi-dimension predictive optimization of engine parameters is performed for the full-cycle engine thermodynamics and the fuel system hydrodynamics. A multi-zone fuel spray combustion model was used to account for peculiarities of mixture formation in diesel and to optimize combustion. A NOx formation model with detailed chemistry is used to handle the combustion effects of massive EGR.
- Multi-dimension optimization of engine parameters was performed at several operating points; the approach to the optimization differs according to the operating point. The contribution of the different operating points to the total emission level of the engine was obtained.
- An equation for objective (target) function calculation which accounts NOx, PM emissions and SFC was proposed.
- A physical split of processes there was performed to decrease the number of variables in a search for an optimum solution. The IVC of the Miller cycle and matching of the piston bowl shape with fuel injector design was in a preliminary optimization. The optimization of compression ratio, nozzle hole diameter, rail pressure and maximum boost pressure and injection profile shape was done at full power operating mode. The optimization of EGR, injection pressure, injection timing and boost control was done at every operating mode.
- The injector design was performed to provide the necessary leading edge rate of injection. The required injection rate was obtained as a result of engine working process optimization. The hydrodynamic simulation tool was used for the injector layout.
- Turbocharger assist offers additional opportunities to improve emissions at part load operating points.
- Control algorithms were identified for the EGR, EGR pump, fuel injection pressure, injection timing and turbocharger assist. The engine performance was predicted together with emissions of NOx and PM as functions of engine speed.
- The results of engine parameters optimization correspond well with published solutions.

# REFERENCES

1. http://ebookbrowse.com/wartsila-w46-pdf-d63675290
2. Dohle U., “MTU solutions for meeting future exhaust emissions regulations,“ Paper No. 284, CIMAC Congress 2010, Bergen, 8 p.
3. Koch F., Seidl T., Schnitzer O., Oehler G., Loettgen A., Loeser S., “Development strategies for high speed marine diesel engines,“ Paper No. 248, CIMAC Congress 2010, Bergen, 9 p.
4. Hopmann U., “Development of the new Caterpillar VM32C LE low emission engine, “ Paper No. 302, CIMAC Congress 2010, Bergen, 7 p.
5. Schlemmer-Kelling U., “The Environment Friendly Medium Speed Engine,” Paper No. 32, CIMAC Congress 2007, Vienna, 10 p.
6. Kendlbacher C., Müller P., Bernhaupt M., Rehbichler G., “Large engine injection systems for future emission legislations,” Paper No. 50, CIMAC Congress 2010, Bergen, 11 p.
7. Heim K., Troberg M., Ollus R., Vaarasto M., “Latest developments in Wärtsilä’s medium-speed engine portfolio,” Paper No. 206, CIMAC Congress 2010, Bergen, 14 p.
8. Andrei Ludu, Michael Engelmayer, Bernhard Pemp, Karl Heinz Foelzer, Thomas Bouche, George Lustgarten, “Large high speed diesels, quo vadis? Superior system integration, the answer to the challenge of the 2012 – 2020 emission limits,” Paper No. 313, CIMAC Congress 2010, Bergen, 2010, 14 p.
9. Malin Ehleskog, Savo Gjirja, Ingemar Denbratt, “Effects of High Injection Pressure, EGR and Charge Air Pressure on Combustion and Emissions in an HD Single Cylinder Diesel Engine,” SAE Technical Paper 2009-01-2815, 2009, 14 p.
10. http://diesel-rk.bmstu.ru

11. A.S. Kuleshov, “Model for predicting air-fuel mixing, combustion and emissions in DI diesel engines over whole operating range,” SAE Technical Paper 2005-01-2119, 2005.
12. A.S. Kuleshov, "Multi-Zone DI Diesel Spray Combustion Model for Thermodynamic Simulation of Engine with PCCI and High EGR Level," SAE Technical Paper 2009-01-1956, 2009.
13. A.S. Kuleshov, A.V. Kozlov, K. Mahkamov, "Self-Ignition Delay Prediction in PCCI Direct Injection Diesel Engines Using Multi-Zone Spray Combustion Model and Detailed Chemistry," SAE Technical Paper 2010-01-1960, 2010.
14. A.S.Kuleshov, “Use of Multi-Zone DI Diesel Spray Combustion Model for Simulation and Optimization of Performance and Emissions of Engines with Multiple Injection” SAE Tech. Pap. Ser. – 2006. – № 2006-01-1385, 2006.
15. Kuleshov A.S. “Multi-Zone DI Diesel Spray Combustion Model and its application for Matching the Injector Design with Piston Bowl Shape” SAE Tech. Pap. Ser. – 2007. – № 2007-01-1908.
16. Kuleshov A.S. “Development of simulation methods and optimization of working processes of ICE” Autoref. Diss. Doct. Tech. Sc. - Moscow, 2011. (in Russian)
17. Bochkov M.V., Zaharov A.U., Hvisevich S.N. “NOx formation at combustion of methane-air mixture in conditions of simultaneous processes of chemical kinetic and molecular diffusion” // Mathematical modeling. – 1997. - Vol 9, N3. – P. 13-28. (in Russian)
18. Grekhov L.V., Ivaschenko N.F., Markov V.F., “Fuel systems and diesel control,” – Moscow, Legion-Autodata, 2005. – 344 p. (in Russian)
19. http://www.iosotech.com/
20. Montgomery David T., Reitz Rolf D., “Optimization of Heavy-Duty Diesel Engine Operating Parameters Using a Response Surface Method,” SAE Technical Paper 2000-01-1962, 2000, 21 p.
21. José M. Desantes, José J. López, José M. García and Leonor Hernández, "Application of Neural Networks for Prediction and Optimization of Exhaust Emissions in a H.D. Diesel Engine," SAE Technical Paper 2002-01-1144, 2002, 10 p.
22. http://www.google.ru/search?q=scania+xpi+injector&hl=en&newwindow=1&prmd=imvns&tbm=isch&tbo=u&source=univ&sa=X&ei=FFuGUPO5COXb4QTMxYCgDg&ved=0CBkQsAQ&biw=1272&bih=736

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## DEFINITIONS / ABBREVIATIONS

| | |
|---|---|
| **A/F** | Air/Fuel equivalence ratio |
| **BMEP** | Brake Mean Effective Pressure |
| **BSN** | Bosch Smoke Number |
| **CR** | Compression Ratio |
| **DI** | Direct Injection |
| **DPF** | Diesel Particulate Filter |
| **EGR** | Exhaust Gas Recirculation |
| **FIE** | Fuel Injection Equipment |
| **HCCI** | Homogeneous Charge Compression Ignition |
| **HRR** | Heat Release Rate, 1/deg |
| **ICE** | Internal Combustion Engine |
| **IVC** | Inlet Valve Close |
| **m_air** | Air mass flow rate, kg/s |
| **NOx** | Nitrogen Oxides, g/kWh |
| **NWF** | Near-Wall Flow |
| **OP** | Opposed Piston (engine) |
| **PCCI** | Premixed Charge Compression Ignition |
| **Pe** | Effective Engine Power, kW |
| **PM** | Particular Mater, g/kWh |
| **PR** | Pressure Ratio |
| **SCR** | Selective Catalyst Reduction |
| **SE** | Total emission |
| **SFC** | Specific Fuel Consumption, g/kWh |
| **SMD** | Sauter Mean Diameter |
| **SN** | Smoke Number |
| **TC** | Turbocharger |
| **Tt** | Temperature at turbine inlet, K |
| s | Fuel fraction in a characteristic zone |

## APPENDIX A

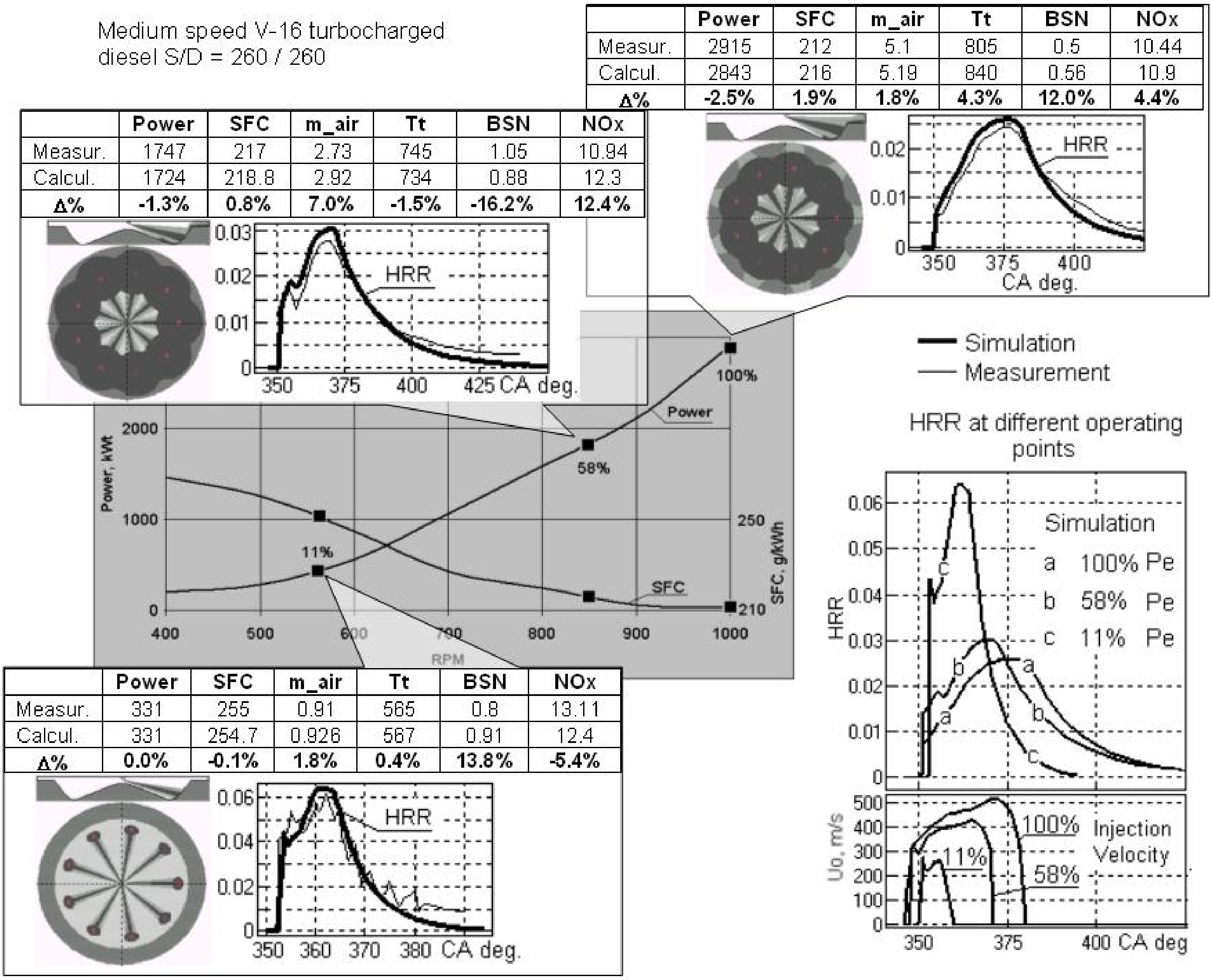


***Figure 16.*** ***Comparison of calculated and measured data of medium speed diesel engine D49 working on locomotive performance.***

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## APPENDIX B

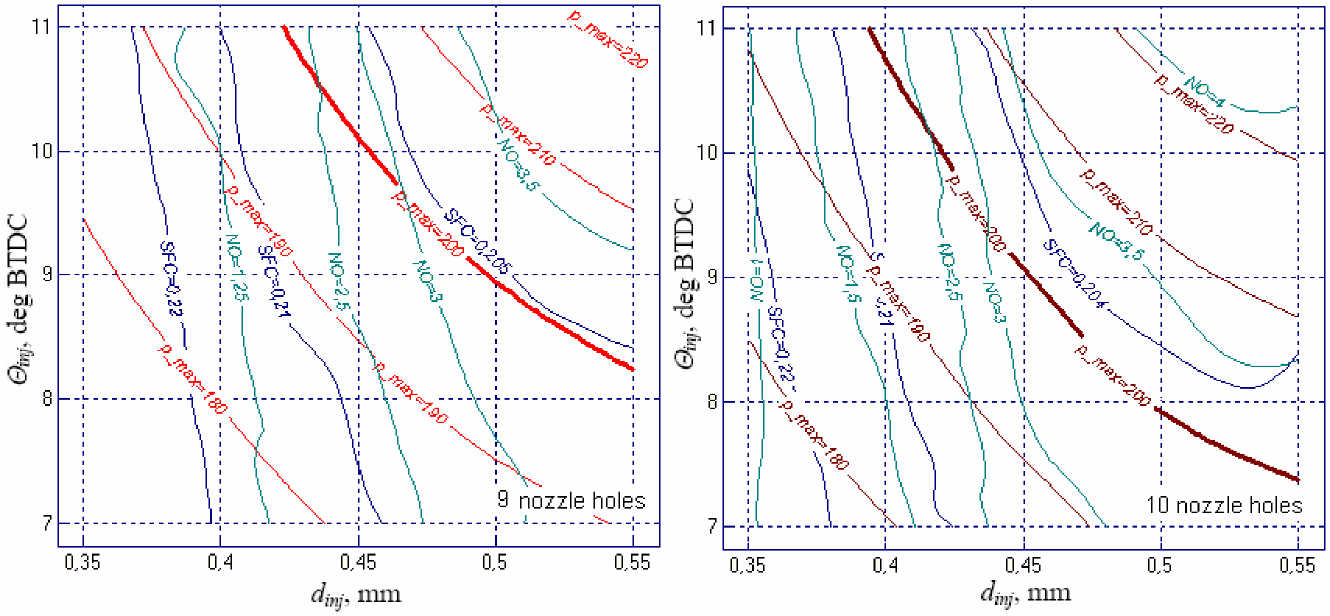


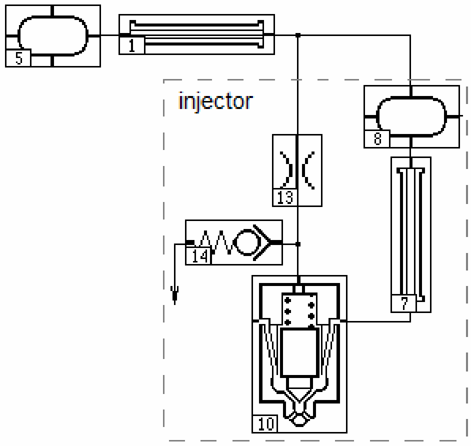

*Figure 17. Effect of nozzles diameter and injection timing on engine parameters at rated power. (With piston bowl "a")*

## APPENDIX C

## Modifications of FIE to approach to injection profile obtained at engine optimization

The injectors of diesels may have an internal accumulator, as it is shown in the Figure 18 a. The volume of the accumulator may exceed a volume of conventional injector in hundred times and one plays important role in shaping the injection profile.


a) Injector of Scania with internal accumulator [22]




b) Simulation scheme of FIE

***Figure 18. Injector with internal accumulator: a) example of design from Scania; b) simulation scheme, where: 5 is Common Rail, 1 is HP pipe, 13 is orifice, 14 is a control valve, 10 is injector, 8 is internal accumulator, 7 is HP bore.***

The injection profile having special shape being derived as a result of engine optimization (Figure 12) was obtained by use wave phenomena in pipe 1, Figure 18 b. To provide the required injection profile there are done following modifications: the internal accumulator 8 is removed and therefore an internal volume of the injector is decreased down to 1000 mm$^3$ (where 500 mm$^3$ is a nozzles volume), the internal diameter of the HP pipe 1 is 3 mm, the effective flow area of orifice 13 is 0.18 mm$^2$, the effective flow area of control valve 14 is 0.25 mm$^2$. All these modifications have provided the approach to the required injection profile by momentary decrease of the fuel pressure before nozzles at the beginning of injection, simultaneously a high pressure is kept in the middle and at the end of injection. The developed injector scheme was used to predict injection profiles at all engine operating points.