Reduction of NOx emissions by numerical optimization of the injection timing for a diesel naval engine

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Abstract: The influence of timing injection on NOx emissions is well known in the literature. If for new engines the requirements imposed by Annex 6 of MARPOL (the document limiting pollutant emissions to ships) are easy to meet, the problem of reducing NOx emissions for in-service engines is a difficult one. The only practical solutions in this situation are to change the injection advance and the injector opening pressure. Practically this is done on the test bench by making adjustments and measurements. This paper aims to analyze this problem using a simulation software developed by the author. The software used simulates the engine cycle without gas exchange processes with the aid of a multidimensional 2.5 D model, completed with phenomenological models for injection modeling. NOx emissions are calculated using a system of 10 equations based on the extended Zeldovich mechanism of which 4 are kinetic and 6 at equilibrium. Complex numerical simulations are presented for the most important operating modes of the chosen engine, performed for different injection timing. The results obtained are compared at the end with the experimental measurements performed on the test bench in order to evaluate the accuracy of the simulations performed and the practical utility of the results obtained to achieve the proposed objective.

Keywords: injection timing, numerical simulations, NOx mechanism, gazodynamic model, fluid-particle interaction.

1. Introduction
The problem of noxious emissions from ships is a very complicated one and solving it involves many technical and financial aspects. Compliance with the rules imposed by Annex 6 to MARPOL (the document governing polluting emissions from ships) for new ships is not a particularly difficult issue given that the rules in the naval field are less restrictive than those in the automotive field. The major challenge is the old ships in operation. The duty cycle for a ship is about 25 years, so they cannot be easily replaced by newer ones when they do not comply with the emission standards.

The compromise solution is to modify the existing engines in operation, so to be able to satisfy partially the existing regulations, many of them being unclassified. The easiest solution to apply is to optimize the injection timing and injector opening pressure so that the engine complies with one of the existing emission standards. Over the last years the influence of injection timing on pollutant emissions has been studied experimental and using simulation software [1], [2], [3]. Among the most popular software we mention the 1-D multizonal software (Wave, AVL Workbench, GT-SUIT, ...) as well, the more complex multidimensional 3D software (KIVA, Vectis, AVL Fire, Ansys Fluent, Forte, ...).

This paper aims to use a multidimensional 2.5 D simulation program developed by the author improved and tested in various conditions over the last years [4], [5]. It has superior performance to 1D software but in many cases inferior to 3D multidimensional. The simulations performed aim to simulate the injection characteristic for the studied naval engine in different speed and load conditions in order to determine the optimal injection timing that minimizes NOx emissions without particularly affecting
the engine performance parameters. The purpose of the simulation is to reduce the number of
adjustments and measurements made on the engines in operation because they are made in difficult
conditions and with high costs.

2. Theoretical background

The code developed by the author and used for the study is a multidimensional one. The formulation
is spatially two-dimensional 2.5 D and allows the plane and axially symmetrical approach of the
combustion chamber geometry.

The realized code solves the systems of specific combined equations for:

- turbulent compressible flow;
- chemical reaction for:
  o fuel oxidation;
  o noxious emissions;
- flow and evaporation of jets composed of liquid particles.

The model governing equations, written in polar coordinates (R polar radius) are briefly presented
below. These have been presented in detail in several other works of the author, with the related
improvements introduced over the years [2], [3]:

The continuity equation for a chemical species

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = \nabla \cdot \left( \rho \mathbf{D} \right) + \rho_s \delta_{t_i}, \quad (1)
\]

where \(D\) is the diffusivity of the species assumed to be the same for all species, \(\rho_s\) is the rate of \(\rho_k\) change due to chemical reactions to be defined later, \(\rho_{t_i}\) is the rate of change of \(\rho_t\) (density of fuel vapor) due to evaporation or condensation of the droplets that make up the fuel jet.

The momentum equation for mixed fluid is:

\[
\frac{\partial (\rho u)}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \left( \rho \mathbf{u} \mathbf{R} \right) \cdot \left( \frac{\sigma_0 - \rho w^2}{R} \right) \mathbf{u} \mathbf{R} + F + \rho G, \quad (2)
\]

where \(p\) is fluid pressure, \(w\) is the swirl velocity (velocity orthogonal on xOy plan), \(\sigma\) is the bidimensional tensor of viscous stresses, \(\sigma_0\) is the cylindrical viscous stress (about z axis), \(F\) is the momentum related to volume and time unit transferred by the droplet to the gas mixture, \(G\) is the mass forces.

The angular momentum equation, that allows the calculations of the swirl speed \(w\) is:

\[
\frac{\partial (\rho w)}{\partial t} + \nabla \cdot (\rho w \mathbf{u}) = \frac{1}{R^2} \nabla \cdot (\rho w \mathbf{R} \mathbf{u}) = \frac{1}{R^2} \nabla \cdot (\rho w \mathbf{R} \mathbf{u}) + N, \quad (3)
\]

where \(\tau\) is the swirl stress, \(N\) is the angular momentum (around the symmetry axis) related to the
volume and time unity transferred from the fuel jet.

The internal energy equation:

\[
\frac{\partial (\rho I)}{\partial t} + \nabla \cdot (\rho I \mathbf{u}) = -\nabla P \cdot \mathbf{u} + \nabla \cdot (\rho w \mathbf{u}) + \rho \mathbf{v} \cdot \mathbf{u} + \nabla \cdot \left( \frac{\sigma_0 \mathbf{u} - \rho w^2 \mathbf{R} \mathbf{u}}{R} \right) + \nabla \cdot (\rho \mathbf{R} \mathbf{u}) + \mathbf{R} \cdot \mathbf{C}_E + \mathbf{R} \cdot \mathbf{S}, \quad (4)
\]

where \(I\) is the specific energy of the gas mixture (without chemical energy), \(J\) is the heat flux, \(\mathbf{C}_E\) is
the energy change rate due to chemical reactions and \(\mathbf{S}\) is a source term associated with the interaction
between the fuel jet and the gas mixture.

The generalized jet equation was approached considering a normal distribution law for the
radius of the droplets around the average diameter Sauter. The particles were divided into drop packets
(depending on the available storage space) that contain particles with the same radius. The interaction
between the droplets was neglected, but the interaction between the droplets and the gas phase was
taken into account. The injection of the particles is modeled taking into account the fact that for each
packet of particle we must be known: the packet speed \(u_{pk}\), particle radius \(r_k\) and \(N_{pk}\) number of particle
in the packet, also called a calculation particle or package (the drops/particle were divided into
packages). Considering $K$ the number of computational particles injected in the unit of time, for each computational particle a radius $r_k$ is chosen using a distribution so as to respect the relationship:

$$\sum_{k=1}^{K} m_k = Q \Delta t,$$

where $Q$ is the flow of injected fuel.

The momentum equation, simplified for a particle (fuel drop pack) $k$ is:

$$m_k \frac{d}{dt} u_{mk} = m_k g - \frac{m_k}{\rho_k} \nabla p + D_k(u_g)(u_g - u_{mk}) + f_k,$$

where $m_k$ is the particle mass, $\rho_k$ is the particle density, $D_k(u_g)$ is aerodynamic drag, $u_g$ is the instantaneous gas velocity written as a result of average and turbulent velocity and $f_k$ is the momentum transferred by the gaseous phase to the particle (eq. 2).

Evaporation was treated considering that the particles are spherical and evaporate inside the cell at constant pressure, in a random order to limit the effect of the interdependence of evaporation between the droplet packets. The term chemical source $C_k$ from equation (1) was calculated taking into account 12 species involved in 10 chemical reactions. In order to solve in good conditions that 10 reactions were divided them into two categories according to the reaction rates:

- 4 kinetic reactions (low speed): an oxidation reaction of the dean $C_{10}H_{22}$ (as the diesel fuel was approximated) in a single step and 3 reactions representing the extended Zeldovich mechanism for nitrogen oxide formation;
- 6 equilibrium reactions (very high speed reactions), dissociation reactions of oxygen, hydrogen, nitrogen, carbon dioxide, hydroxyl radical and water.

$$\begin{align*}
2C_{10}H_{22} + 31O_2 & \rightarrow 20CO + 22H_2O \\
O_2 + 2N_2 & \leftrightarrow 2N + 2NO \\
2O_2 + N_2 & \leftrightarrow 2O + 2NO \\
N_2 + 2OH & \leftrightarrow 2H + 2NO \\
O_2 + H_2 & \leftrightarrow 2OH \\
O_2 + H_2O & \leftrightarrow 4OH \\
O_2 + 2CO & \leftrightarrow 2CO_2 
\end{align*}$$

The numerical scheme is solved using a partially implicit algorithm with advance in steps of time, using a finite volume discretization scheme.

The discretization mesh is adjustable and consists of generalized quadrilaterals whose corners are specified by time-dependent coordinates relative to the lower position of the piston, which allows the Eulerian or Lagrangean approached of the problems as needed.

For wall conditions, uniform laws were used for the jacket, piston and cylinder head, with the difference that the wall represented by the piston is movable.

The implemented algorithm allows differentiated approach of the wall flow as follows:

- free slip flow;
- no slip flow;
- flow with turbulent law at the wall.

For the wall heat exchange the cases were implemented is:

- constant wall temperature, fixed prescribed on the entire contour of the combustion chamber;
- adiabatic walls, without heat exchange.

The developed code does not fully model the processes cycles in the engine, only those without gas exchange: compression, combustion and expansion, but the program was built to allow further developments, using the already written modules.

In order to pass the simulation requirements imposed by solving the proposed problem, the program developed by the author was completed with a special module to assess the friction lost power using Heywood's formulas [6]. For this, it was considered that the in-cylinder work per cycle is calculated precisely from the processes without gas exchange modeled by the code and then the work from processes whit gas exchange is add. For simplicity the processes whit gas exchange is considered at constant pressure.
The calculation program was originally written in MATLAB after which it was transferred into FORTRAN for a higher calculation speed and a more efficient management of computer resources.

3. Experimental measurements
The engine chosen for optimization was the T680, a 4-stroke non-supercharged naval engine produced by Tractorul Brașov. It is not very representative for the naval field, but it is frequently encountered on board of technical ships in Diesel-generating groups. This engine is very widespread and small in size so it could be tested on the test bench. The testing on the test bench allow to take many measurements with high accuracy. The measurement on board ships are inaccurate and it is very difficult achieve.

Annex 6 of MARPOL regulates NOx emissions from ships, imposing limits for specific weighted emissions measured over a 8-Mode C1 cycle. Optimizing NOx emissions means minimizing specific weighted emissions without affecting too much the engine performance. The 8-Mode emissions cycle requires the measurement of NOx emissions at maximum power and maximum torque speeds.

In order to study the effect of the injection timing on NOx emissions, many measurements were made for several regimes with different values of the injection timing. The real injection timing was determined experimentally, using the needle lift diagram for the first injector at idle speed. The most significant measurements performed and processed according to the methodology presented in Annex 6 of MARPOL, are that for the nominal power speed and maximum torque speed at full load. The values are shown in figures 1 and 2.

The real initial injection timing angle was 6.5° CAR (crank angle rotation) and from the graphic analysis it can be seen that the optimal value of the injection advance would be 4.5° CAR. Advance This value has been chosen so that we do not have a decrease of more than 2% for the nominal engine power and in particular an increase of consumption.
For validation, noxious cycles were performed for injection timing around 4.5° CAR. Figure 3 contains the variation with the injection timing for the weighted average of NOx specific emissions, achieved with the 8-Mode C1 cycle, recommended by Annex 6 of MARPOL. In the table 1 are the values for the weighted average specific emissions at injection timing of 4.5° CAR.

**Table 1 Weighted average of pollutant specific emissions at 4.5° CAR injection timing**

| Load [%] | Speed [rpm] | 8-Mode C1 | NOX*wfi [g/h] | CO*wfi [g/h] | tHC*wfi [g/h] | P*wfi [kW] |
|----------|-------------|-----------|---------------|---------------|---------------|-------------|
| 100      | 2400        | 0.15      | 57.8462       | 28.0427       | 7.551         | 4.7557      |
| 75       | 2400        | 0.15      | 41.4193       | 13.3975       | 7.913         | 5.658       |
| 50       | 2401        | 0.15      | 30.5939       | 15.6558       | 7.791         | 3.764       |
| 10       | 2404        | 0.1       | 9.8169        | 15.5406       | 6.2538        | 0.516       |
| 100      | 1440        | 0.1       | 29.7511       | 11.5739       | 1.6677        | 3.452       |
| 75       | 1439        | 0.1       | 22.7687       | 3.1454        | 2.2111        | 2.606       |
| 50       | 1439        | 0.1       | 18.8759       | 3.1102        | 2.6959        | 1.726       |
| 0        | 812         | 0.15      | 4.5135        | 2.2201        | 0.9431        | 0.000       |
| SUM=     |             |           | 215.5854      | 92.6862       | 33.2765       | 25.279      |

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| Annex 6 MARPOL | NOX [g/kWh] | CO [g/kWh] | tHC [g/kWh] |
|----------------|-------------|------------|-------------|
| 9.2            | 6.5         | 1.3        |

### 4. Numerical results

In order to perform the numerical simulation of the noxious cycle, we initially propose to calibrate the model at the nominal speed because for an engine this is the speed for which we have the most data. For naval engines the existing documentation on board is more detailed than for car engines and in addition we have indicated diagrams taken on board. The only major problem is setting the real injection timing, because normally only the adjustment injection timing is known. The solution applied was to consider the actual injection timing angle that is obtained when turning the engine until the moment when fuel appears at the nozzle holes of an injector removed from the cylinder head. This value for the considered engine was very close to that determined by measurements at idle speed.

Calibration simulations are performed for maximum power speed and load 100%: the speed is 2400 rpm, the effective power is 52 kW, the effective torque is 206 Nm, the specific consumption is 238 g / kWh and the effective injection timing is 6.5° CAR.
For a better interpretation of the obtained data, a calculation model was developed using the specialized program Wave 5.0 by Ricardo. This program offers users only mono and multizone thermodynamic models, improved with phenomenological models especially for modeling fuel jets. The chosen model is the most complex of those existing in the program database. It is a multi-zone model that is based on layered fuel jet modeling. It was mainly used for the primary evaluation of the parameters of the noxious cycle regimes, the specific fuel consumption and the effective power at a certain speed and injection timing. This program has the advantage of a very short working time compared to the multidimensional one developed by the author. The obtained parameters were used as input data for the multidimensional model and thus greatly reduced the working time.

The calibrations were performed mainly on the basis of the indicated diagram. Successive corrections were made until the best possible correspondence was obtained between the indicated measured diagram and those calculated with the two simulation programs. At the end, the emissions model was also calibrated, by comparing it with the measured average values. The final result is shown in figures 4, 5, 6, 7 and 8.

With the calibrated models, calculations are performed to determine the dependence of NOx emissions on the injection timing. The main important results are presented in table 2.

![Figure 4: Pressure at 2400 rpm speed and load 100%](image1)

![Figure 5: NOx concentration at 2400 rpm speed and 100% load](image2)

![Figure 6: Pressure at 1440 rpm speed and load 100%](image3)

![Figure 7: NOx concentration at 1440 rpm speed and 100% load](image4)
It is observed that with the decrease of the injection timing, the NOx emissions also decrease, but the effective engine power is also reduced. For this reason, a limit of effective power reduction of maximum 2% is imposed, as in the case of experimental determinations. With this limit imposed in table 2 it can be deduced that the optimal injection timing would also be 4.5° CAR to reduce pollutant emissions, without greatly affecting engine performance.

The results of the calculation of an 8-Mode C1 emissions cycle for the 4.5° CAR injection timing are shown in table 3.

### 5. Conclusions

Experimental measurements on the test bench have shown that it is possible to reduce NOx emissions by modifying the injection timing so that the engine falls within the emission limits prescribed by Annex 6 MARPOL, the problem is the decreased performance. The decrease in effective power and the increase in fuel consumption accompanied by the increase in smoke emissions is the main drawn back. It should be noted that the tests were performed using automotive Diesel fuel, which is different from marine Diesel fuel which have not additive and for this reason the engine performance is negatively affected, effective power decreases and smoke emissions increases.

The results obtained from the measurements and those calculated with the program are in good concordance. For the conditions imposed, the optimal injection timing angle was correctly estimated.

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### Tab. 2 NOx concentration according to injection timing

| Speed [rpm] | Timing [deg] | NOx [ppm] | NOx-calc [ppm] | Error [%] | Power [kW] |
|-------------|--------------|-----------|----------------|-----------|------------|
| 2400        | 3.5          | 732       | 776            | 6.01      | 47.64      |
|             | 4            | 796       | 858            | 7.79      | 48.34      |
|             | 4.5          | 850       | 929            | 9.29      | 49.82      |
|             | 5            | 964       | 1056           | 9.54      | 51.4       |
|             | 5.5          | 1008      | 1101           | 9.23      | 51.62      |
|             | 6            | 1112      | 1185           | 6.56      | 51.89      |
|             | 6.5          | 1134      | 1218           | 7.41      | 52.17      |
| Rezultat    | 3.5          | 1156      | 1232           | 6.57      | 33.12      |
|             | 4            | 1221      | 1321           | 8.19      | 33.81      |
|             | 4.5          | 1344      | 1455           | 8.26      | 34.21      |
|             | 5            | 1498      | 1573           | 5.01      | 34.52      |
|             | 5.5          | 1557      | 1643           | 5.52      | 34.78      |
|             | 6            | 1614      | 1732           | 7.31      | 34.91      |
|             | 6.5          | 1687      | 1821           | 7.94      | 34.96      |
The only problem remains the increase of smoke emissions. For this concrete case studied where no differences.

Tab. 3. Calculated weighted average of pollutant specific emissions at 4.5° CAR injection timing

| NOX [g/h] | CO [g/h] | Load [%] | Speed [rpm] | 8 Mode C1 | NOX\*wfi [g/h] | CO\*wfi [g/h] | P\*wfi [kW] |
|-----------|---------|----------|-------------|-----------|----------------|----------------|-------------|
| 421.4834  | 175.8068| 100      | 2400        | 0.15      | 63.2225        | 26.3710        | 7.473       |
| 285.3957  | 71.7529  | 75       | 2400        | 0.15      | 42.8094        | 10.7629        | 5.605       |
| 211.9820  | 92.6703  | 50       | 2400        | 0.15      | 31.7973        | 13.9005        | 3.737       |
| 112.0397  | 178.7150 | 10       | 2400        | 0.1       | 11.2040        | 17.8715        | 0.498       |
| 322.0825  | 131.9192 | 100      | 1440        | 0.1       | 32.2082        | 13.1919        | 3.421       |
| 242.7450  | 29.5255  | 75       | 1440        | 0.1       | 24.2745        | 2.9526         | 2.566       |
| 200.9459  | 27.4730  | 50       | 1440        | 0.1       | 20.0946        | 2.7473         | 1.711       |
| 31.6791   | 10.8823  | 0        | 800         | 0.15      | 4.7519         | 1.6323         | 0.000       |

SUM= 230.3623 89.4301 25.0097

| NOX [g/kWh] | CO [g/kWh] |
|------------|------------|
| 9.2109     | 3.5758     |

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Anexa 6 MARPOL
9.2
6.5
9.8

but this must be carefully verified for each engine separately. The problem of the injection timing angle introduced as initial data in the calculation program is a great challenge that differs for each regime and is not constant. Measured values are welcomed but is hard to achieve in exploitation conditions. The maximum error between the calculated and the estimated values is 10%. This is mainly due to the error in estimating:

- NOx emissions that has a maximum of 9.3% as shown in table 2, the NOx concentration is constantly overestimated by the program;
- cumulative error in calculating the weighted average NOx specific emissions per 8-Mode C1 cycle that has a maximum of 8% (tables 1 and 3);
- effective power that has a maximum error of -1.1% (tables 1 and 3);

The final conclusion is that we can optimize NOx emissions according to the injection time using the numerical simulation program, but we must be careful. The estimated error is not very small, but the reserve at the value of 9.8 [g / kWh] recommended in Annex 6 MARPOL is covering (tables 1 și 2).

In order to increase the performance of the simulation program, it should mainly contain a module for estimating smoke emissions which plays an important role in estimating engine emissions and an even phenomenological module that can connect the mounting injection timing to the real one.

References
[1] S. Emami, S. Jafarmadar, Multidimensional modeling of the effect of fuel injection pressure on temperature distribution in cylinder of a turbocharged DI diesel engine, Propulsion and Power Research, 2 (2013), pp. 162-175
[2] Ishiwata, H., Ohishi, T., Ryuzaki, K., Unoki, K. et al., A Feasibility Study of Pilot Injection in TICS (Timing and Injection Rate Control System), SAE Technical Paper 940195, 1994, https://doi.org/10.4271/940195.
[3] O'Donnell, P., Rahimi Boldaji, M., Gainey, B., and Lawler, B., Varying Intake Stroke Injection Timing of Wet Ethanol in LTC, SAE Technical Paper 2020-01-0237, 2020, https://doi.org/10.4271/2020-01-0237.
[4] Sabău A., Pressure waves simulation in Diesel engine injection system, Modern Technologies in Industrial Engineering (2013), Sinaia, Vol. 837 of Advanced Materials Research, pp 476-482, ISSN web 1662-8985
[5] Sabău A., Pressure Injection Influence on the Combustion Process, International Conference on Advanced Concepts in Mechanical Engineering II (2014), Iasi, Applied Mechanics and Materials Vol. 659 pp 450-455, ISBN: 978-3-03835-272-3

[6] Heywood, John E., Internal Combustion Engine Fundamentals, Published by MCGRAW-HILL Higher Education (1989), ISBN 10: 0071004998 ISBN 13: 9780071004992