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Measurement and simulation of pollutant emissions from marine diesel combustion engine and their reduction by exhaust gas recirculation †

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Abstract

Taking into account the complexity and cost of a direct experimental approach, the recourse to simulation, which can also predict inaccessible information by measurement, offers an effective and fast alternative to apprehend the problem of pollutant emissions from internal combustion engines. An analytical model based on detailed chemical kinetics employed to calculate the pollutant emissions of a marine Diesel engine in general gave satisfactory results compared to experimentally measured results. Especially, the nitric oxide (NO) emission values were found to be higher than the limiting values tolerated by the International Maritime Organization (IMO). Thus, this study was undertaken to reduce to the maximum these emissions. The reduction of pollutant emissions is apprehended with exhaust gas recirculation (EGR).

Keywords: Engine combustion; Numerical modeling; NOx and SOx emissions; Detailed chemical kinetic

1. Introduction

The energies produced by the diesel engines of strong power are largely used in marine propulsion, because of their favorable reliability and their significant output. However, the increasingly constraining legislations, aimed at limiting the pollutant emissions from the exhaust gas produced by these engines, tend to call into question their supremacy [1, 2].

Many studies have been undertaken, as well on the experimental level as on the analytical level, in order to study the mechanisms which govern the formation of the various produced pollutants [3-5]. The analysis of the pollutant emissions and their reduction in the exhaust gas of the semi-rapid turbocharged marine diesel engine constitutes the principal objective of this study.

With advanced research, it is still impossible, in combustion, to treat at the same time complex kinetics and industrial turbulent flow conditions. The majority of the studies treated the detailed chemistry of combustion in association with ideal flow reactor conditions [5, 6]. The various simulations carried out in this work are based on the computer code marketed by Reaction Design, the CHEMKIN package, which is developed by the Sandia laboratories.

Comparisons of the numerical predictions with the experimental results carried out on a real unit at use aboard a car ferry ship made it possible to analyze the validity of the numerical results.

2. Experimental study

The unit selected for measurements is a power generating unit in use on a car ferry ship during its docking in a harbor. The diesel engine unit is a WARTSILA NSD type 6R32 LNE having characteristics by given in Table 1 with a nominal power of 2460 kW. The measured values taken in exhaust gas were carried out using a Testo350 (Precision +/- 5 %

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Table 1. Characteristics of the diesel engine of the power generating unit.

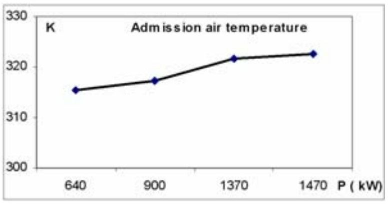
Firing order	1-5-3-6-2-4
Speed	750 tr/mn
Piston speed	8,4 – 8,8 m/s
Cylinder bore	32 cm
Piston stroke	35 cm
Connecting rod lengh	74,5 cm
Compression ratio	12
Effective mean pressure	28,5 Bar
Maximal firing pressure	165 Bar
Clearence volume	2557,7 cm 3
Injection pressure	450 Bar

m.v) gas analyzer. which made it possible to post with precision and in real time the percentage by volume of oxygen (O_2), percentage by volume of carbon dioxide (CO_2), nitric oxide (NO), sulfur dioxide (SO_2), temperature and pressure.

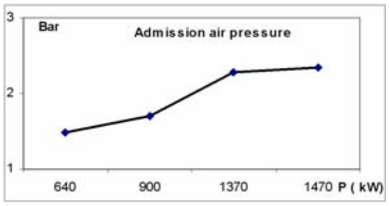
The measurements were carried out for various powers: 640, 900, 1370 and 1470 kW.

To determine the emitted quantities in grams per cycle per cylinder (g/cyc/cyl) and in (g/kWh) it is necessary to deduce the volume (V_m) of the exhaust gas at the measurement point at atmospheric pressure (P_a) and for exhaust gas temperature (T_m):

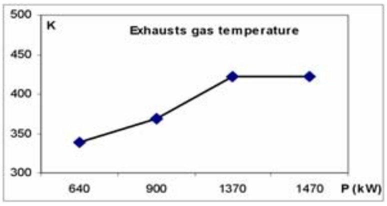
$$V_m = \frac{m_T R_g T_m}{P_a} \tag{1}$$



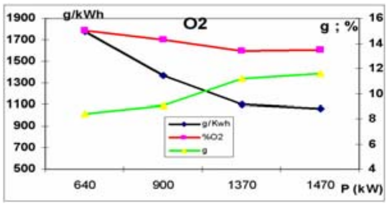
(a) Evolution of admission air temperature



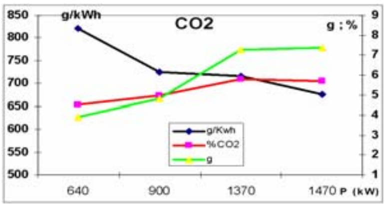
(b) Evolution of admission air pressure



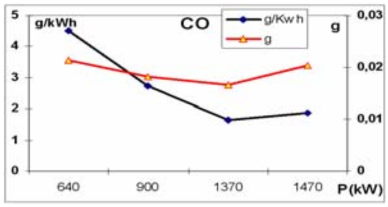
(c) Evolution of exhaust gas temperature



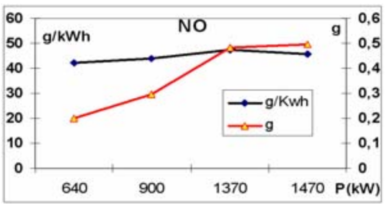
(d) O2 Evolution



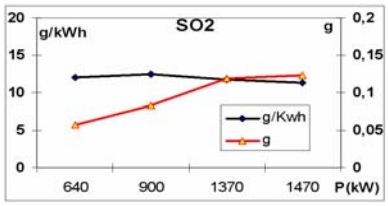
(e) CO2 Evolution



(f) CO Evolution



(g) NO Evolution



(h) SO2 Evolution

Fig. 1. Parameters measured with gas analyzers.

where the volume is calculated from the ideal gas equation of state. The mass conservation law enables us to deduce the mass with the admission condition :

$m_T = m_{air} + m_{comb}$
where it is assumed $m_{air} = 15\ \lambda_a\ m_{comb}$ (2)

The volume of exhaust gas at the measurement point is then:

$$V_m = V_{cyl} \frac{T_m}{T_{adm}} \frac{P_{adm}}{P_a} (1 + \frac{1}{15\lambda_a}) \quad (3)$$

Fig. 1 presents the preliminary experimental results obtained on the chosen unit.

As a consequence of the increase in power we note:
- A greater quantity of exhaust gas increasing the mode of the turbocharger and consequently the pressure of air of overfeeding.
- An increase in overfeeding air temperature.
- A decrease in percentage by volume of O_2 with an increase in percentage by volume of CO_2.
- An increase in NO emission.
- An increase in SO_2 emission.

According to these notes, we can conclude that there is an improvement of combustion for the passage from the low power to the semi-maximum power of the generating unit.

The cycle temperature increases causing a higher formation of thermal NO. In addition, the admitted quantity of air is larger and consequently supporting the formation of NO in greater quantity. This last is higher than the allowed NO emission by the IMO.

This initiated our study to reduce the NO emissions of marine diesel engines.

3. Numerical study

It is often difficult to carry out directly a parametric study on a real unit since the study of combustion is generally complex with the simultaneous presence of several physical and chemical phenomena that vary from one model to another according to the aero thermo chemical conditions of the application. For that, it is necessary to be able mathematically to describe the aero thermo chemical phenomena that control the various processes present in a real combustion chamber.

In spite of the high capacity of computers, it is still impossible, in combustion, to treat at the same time complex kinetics and industrial turbulent flow conditions. For this reason, one uses the modelling based on ideal chemical reactors with simplified flows. These reactors are simulated by using several hundreds of reactions [5-7].

Due to the high turbulence in the combustion chamber induced by the admission of overfeeding air through deflectors and the corrugated shape of the piston (with pre chamber) in addition to the injection system (high pressure: 450 to 600 Bar) [8, 9] that allows a good distribution of the fuel jet in the combustion chamber [10-13], one can admit that the reagents mixture is homogeneous, and we assume that the combustion process can be modelled by a perfectly stirred reactor (PSR) [14, 15].

In a PSR, the mixing in the reactor chamber is supposed intense and, thus, it is assumed that the temperature and composition in the reactor are uniform through the reactor volume.

A description of the process occurring within the PSR is obtained by relating the conservation of mass and energy to the generation of chemical species within the reactor volume [6, 16].

The species conservation equation is:

$$\dot{m}(Y_k - Y_k^*) - \dot{\omega}_k M_k V = 0 \quad k = 1,\ldots\ldots\ldots,K \quad (4)$$

The energy conservation equation is:

$$\dot{m} \sum_{k=1}^{K} (Y_k h_k - Y_k^* h_k^*) + Q = 0 \quad (5)$$

The nominal residence time is:

$$\tau = \frac{\rho V}{\dot{m}} \quad (6)$$

Where the mass density ρ is calculated from the ideal gas equation of state:

$$\rho = \frac{P\overline{M}}{R_g T} \quad (7)$$

From this set of (K +1) nonlinear algebraic equations, solutions for the temperature and mass fractions are obtained. Even though one seeks the solution to the steady-state equations, the computational algorithm often requires a partial solution of the related transient problem.

The analogous time-dependent equations for mass conservation of each species are:

$$\frac{dY_k}{dt} = \frac{-(Y_k - Y_k^*)}{\tau} + \frac{\dot{\omega} M_k}{\rho} \quad (8)$$

and the time-dependent energy conservation equation is:

$$C_p \frac{dT}{dt} = \frac{1}{\tau}\sum_{k=1}^{K} Y_k^* (h_k^* - h_k) - \sum_{k=1}^{K} (\frac{h_k M_k \dot{\omega}_k}{\rho}) - \frac{\dot{Q}}{\rho V} \quad (9)$$

The net chemical production rate $\dot{\omega}_k$ of each species results from a competition between all the chemical reactions involving that species. Each reaction proceeds according to the law of mass action and the forward rate coefficients (k_f) are in modified Arrhenius form:

$$k_f = AT^{\beta} \exp\left(\frac{-E_A}{R_g T}\right) \quad (10)$$

The simulation of the internal combustion with high turbulent conditions of an engine is carried out by the CHEMKIN code using 450 elementary reactions mechanism between 77 species including the sulfur (case of the fuel oil). Specifically, the model ICEM (internal combustion engine model) has been used to simulate the temporal behavior of the engine combustion [16].

The process of ignition of fuel used by the code is governed by its temperature of auto ignition.

The relation between volume swept by the piston divided by clearance volume is:

$$\frac{V_{cyl}}{V_0} = 1 + \frac{C-1}{2}\left[G + 1 - \cos\alpha - \sqrt{G^2 - \sin^2\alpha}\right] \quad (11)$$

The convective heat transfer coefficient between the gas and cylinder wall obtained from the generalized heat transfer correlation in terms of a Nusselt number Eq. (12) and Eq. (13).

$$Nu_h = a\, Re^b Pr^c \quad (12)$$

$$Nu_h \equiv \frac{hS}{\lambda} \quad (13)$$

The heat loss is calculated at each step in time according to:

$$Q_{\text{wall}} = hS\,(T - T_{\text{wall}}) \quad (14)$$

The Woschni correlation [16] allows a more accurate estimation of the average cylinder gas speed used in the definition of the Reynolds number for the heat-transfer correlation.

The velocity used in the Reynolds number definition in Eq. (15) is an estimation of the average cylinder gas velocity, Z, instead of the mean piston speed.

$$R_e \equiv \frac{D\bar{Z}\rho}{\mu} \quad (15)$$

To obtain the average cylinder gas velocity, Woschni proposed a correlation that relates the gas velocity to the mean piston speed and to the pressure rise due to combustion:

$$Z = \left[C_{11} + C_{12}\frac{v_{swirl}}{\bar{S}_p}\right]\bar{S}_p + C_2\frac{V_d T_i}{P_i V_i}\left(P - P_{motored}\right) \quad (16)$$

The chosen composition of species weight of the fuel introduced in the code is composed of 86.6 % in mass of carbon, 10.9 % in mass of hydrogen and 2.5 % in mass of sulfur.

The numerical results are established according to pressure, which varies from 1.7 to 2.35 Bar, an overfeeding air temperature which varies from 317 to 322 K, and an equivalence ratio which varies from 0.6 to 0.8, corresponding to the values measured with the powers which vary from 900 to 1470 kW and for an ambient temperature of 306 K.

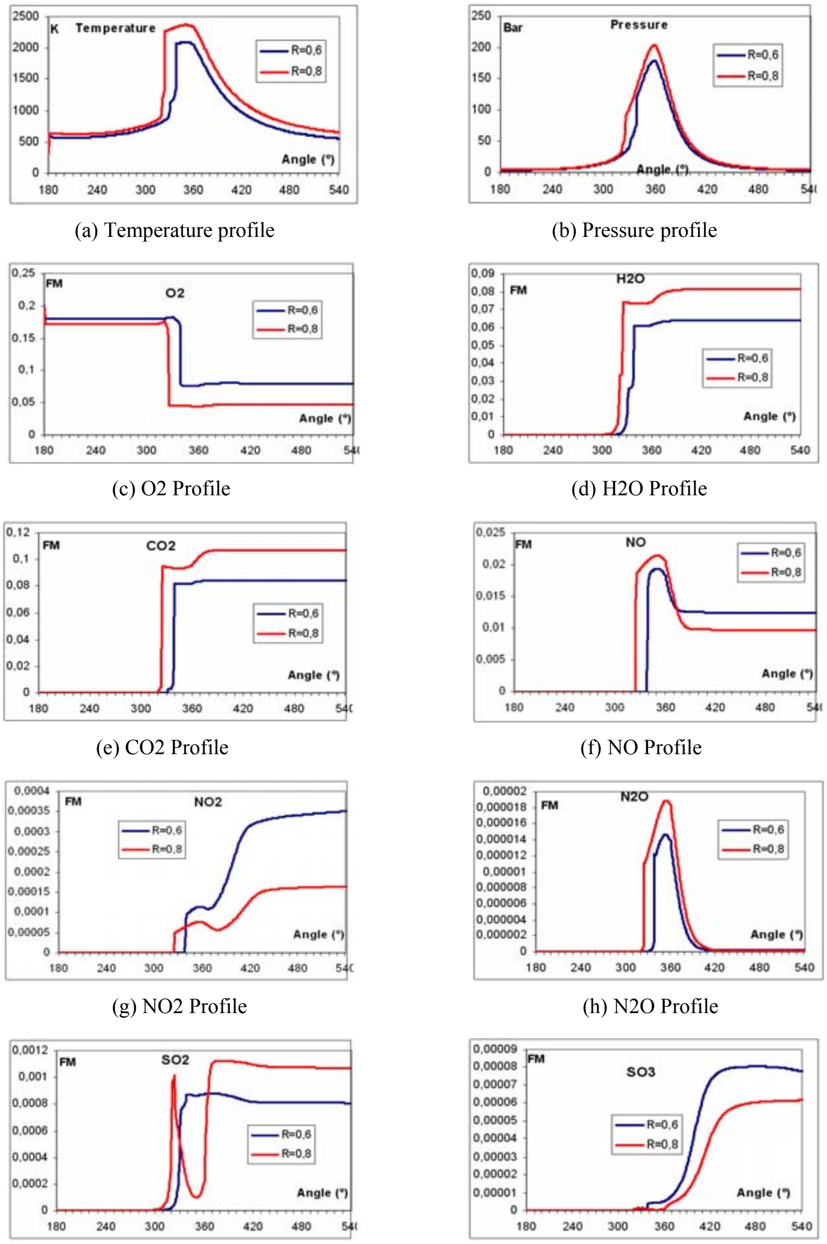
The first objective of the study was to analyze the influence of the equivalence ratio on the course of the combustion process and on the pollutant emissions related to the real engine conditions (overfeeding air temperature, overfeeding air pressure, engine speed, …).

The numerical conversion of the results MF (Molar Fraction) into grams (m_k) Eq. (17), for each species k (k varying from 1 to 77) is obtained while passing by the molar masses M_k and the total mass $m_T = \sum_{k=1}^{77} m_k$

$$m_k = m_T \frac{M_k MF_k}{\sum_{k=1}^{77} M_k\, MF_k} \text{ in grams} \quad (17)$$

Fig. 2 illustrates the influence of the equivalence ratio on the progress of the combustion and the pollutant emissions according to the crank rotation angle. The observed jump of the parameters corresponds to the beginning of the combustion which starts, with an advance, with regard to the piston top dead center (360°) and with a delay of ignition which varies with the equivalence ratio.

For a reduction in the equivalence ratio (from R= 0.8 to R=0.6) we note that the excess of total air leads to dilute exhaust gas which decreases its temperature and pressure, an increase in the ignition delay, a decrease in the total time of combustion, a considerable increase in NO as of NO_2 and SO_3 emissions, a considerable decrease in H_2O, SO_2 and CO_2 emissions. We conclude that there is an improvement in the



(a) Temperature profile
(b) Pressure profile
(c) O2 Profile
(d) H2O Profile
(e) CO2 Profile
(f) NO Profile
(g) NO2 Profile
(h) N2O Profile
(i) SO2 Profile
(j) SO2 Profile

Fig. 2. Evolutions of the temperature, the pressure and the pollutant emissions in the combustion chamber.

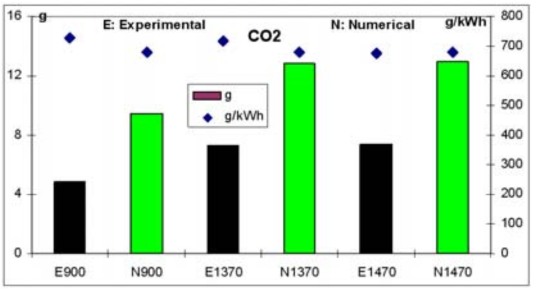


Fig. 3. Evolution of numerical and experimental results for the CO2 emission

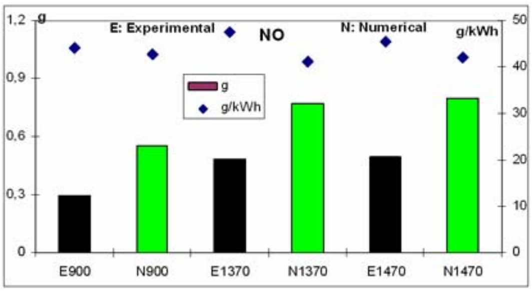


Fig. 4. Evolution of numerical and experimental results for the NO emission.

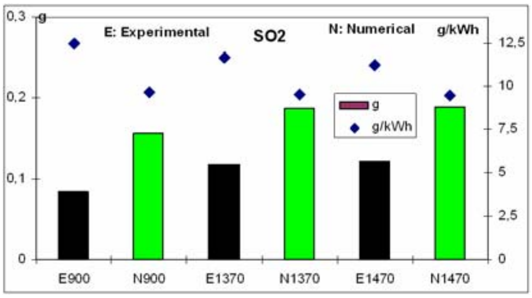


Fig. 5. Evolution of numerical and experimental results for the SO2 emission.

combustion process.

The considerable increase in the excess of air and consequently that of atmospheric nitrogen support the formation of NOx in quantity to the exhaust gas which increases.

For a poor mixture the fuel jet of a smaller quantity of fuel undergoes a faster oxidation, which has as a consequence an increase in the time of ignition.

The different values expressed in g/cycle/cylinder and g/kWh are given by considering a low calorific value of 42.000 kJ/Kg and a total output of 0.4 .

The content of COx is made up mainly of 99.9 % to CO_2.

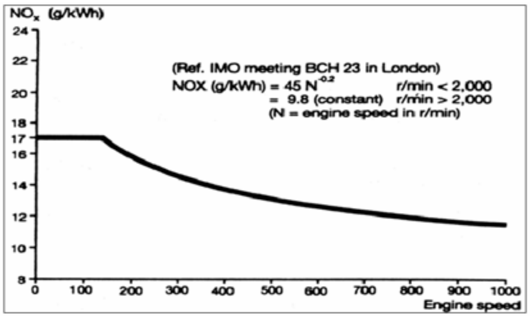


Fig. 6. Curve IMO limiting the NOx emissions according to the nominal speed of the engines [17].

The content NOx is made up mainly of 97.5% in NO and 2.5% in NO_2 in the poor mixture; consequently, the NOx emission undergoes an increase since it follows the same evolution of the majority species which is the NO.

The content of SOx is made up mainly of 95% of SO_2 and 5% of SO_3 in the poor mixture; consequently, the emission of SOx undergoes a small decrease.

Figs. 3-5 show comparisons between computed and measured CO_2, NO and SO_2 emitted quantities in the exhaust gas as a function of engine power.

Relatively good agreements are observed especially for emission expressed in g/kWh. One can conclude that the model of the adopted calculation allows qualitative and quantitative results, that are, in general, satisfactory. But it should be well noted that the precision of the results depends on the adequate determination of the precision of measures and the assumption adopted in the model.

Fig. 6 shows the IMO [17] curve for the limiting NOx emissions according to the nominal speed of the engine. For a speed of 750 rpm, the NOx is limited to a value of 12.2 g/kWh.

All the values of NO (g/kWh) in Fig. 1.g, and for the various powers, are higher than the limiting value tolerated by the IMO.

4. Study of exhaust gas recirculation

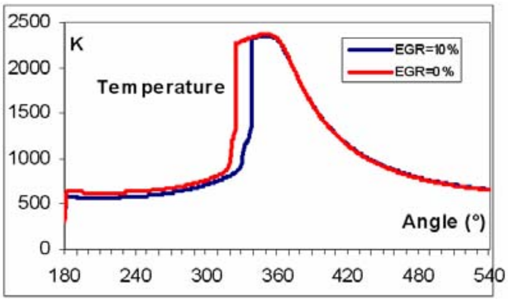
Therefore, a subsequent study has been done to reduce this NO emission [18-20] by exhaust gas recirculation.

The objective of this study was to analyze the influence of EGR [21, 22] in the combustion chamber of the diesel engine on the different pollutant emissions.

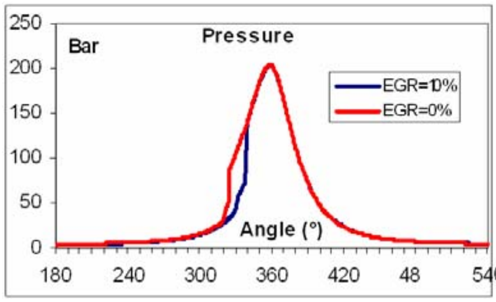
The study of influence of EGR is that corresponding to the measured maximum power (1470 kW) having a temperature of admission air of T_a= 322 K and a pressure of admission air of P_a = 2.35 Bar.

The numerical results are established according to H_2O mass in reagent, which varies from 0 to 1.13 g, a CO_2 mass which varies from 0 to 2.85 g, and for air mass which varies from 74.38 to 70.57 g.

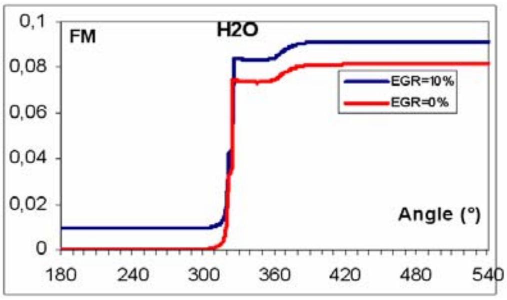
The volume of exhaust gas mixed with the admis-



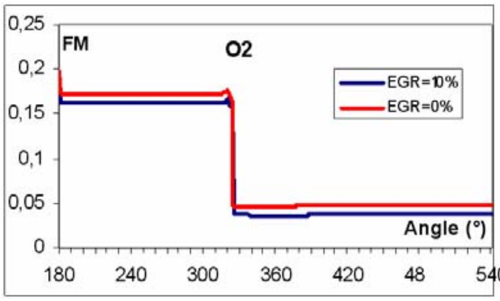
(a) Temperature profile



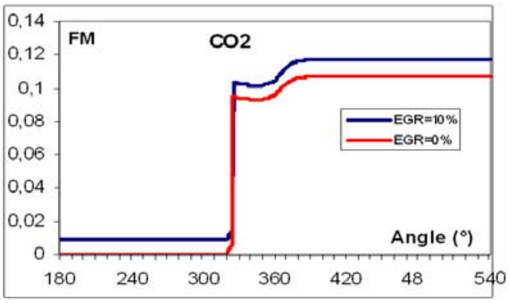
(b) Pressure profile



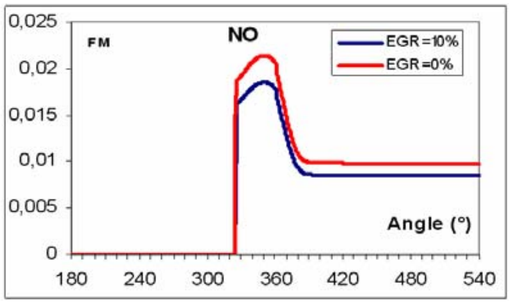
(c) H2O Profile



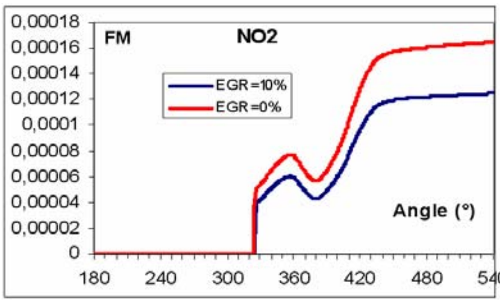
(d) O2 Profile



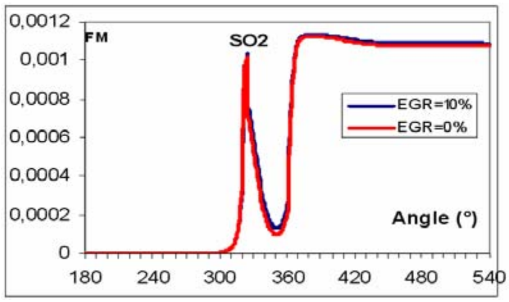
(e) CO2 Profile



(f) NO Profile



(g) NO2 Profile



(h) SO2 Profile

Fig. 7. Evolutions of the temperature, the pressure and the pollutant emissions.

sion air is:

$$V_{EGR} = \frac{Z_{EGR} V_{Cyl}}{100} \quad (18)$$

and $$V_{air} = \frac{(100 - Z_{EGR}) V_{Cyl}}{100} \quad (19)$$

The temperature of the mixture before turbocharger is:

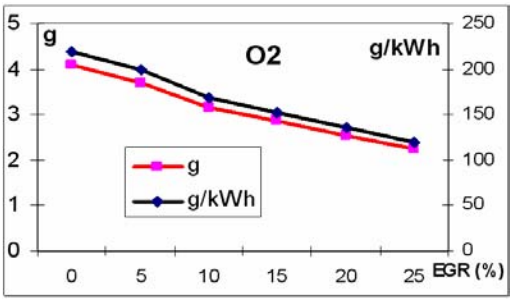
$$T_{mix} = \frac{\frac{V_{air}}{r_{air}} c_{p_{air}} + \frac{V_{EGR}}{r_g} c_{p_g}}{c_{p_{mix}} \left(\frac{V_{air}}{r_{air} T_{air}} + \frac{V_{EGR}}{r_g T_g} \right)} \quad (20)$$

The volume of the exhaust gas is:

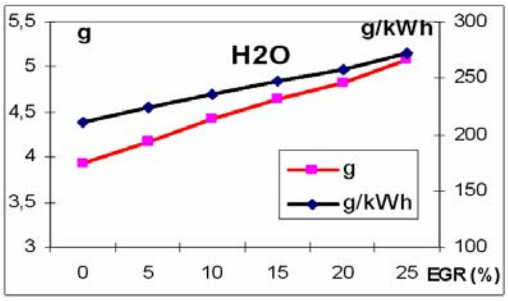
$$V_g = r_g T_g \left(\frac{P_{adm} V_C}{r_{mix} T_{adm} P_a} + \frac{m_{comb}}{P_a} \right) \quad (21)$$

Fig. 7 illustrates the influence of exhaust gas recirculation on the course of combustion and the pollutant emissions. It represents the variations of pressure, temperature and NO and SO_2 in the cylinder as a function of the crank rotation angle with and without EGR. A substantial reduction in NO and NO_2 emissions and an increase in the ignition delay and CO_2 emission are noted. The SO_2 emissions remain constant.

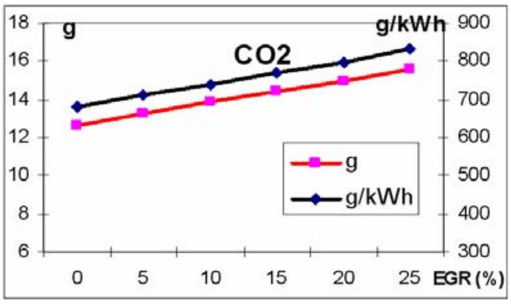
Fig. 8 illustrates the influence of exhaust gas recir-



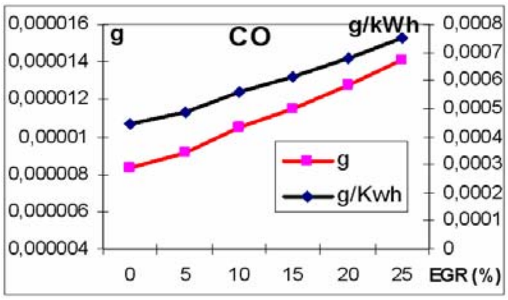
(a) O2 mass evolution



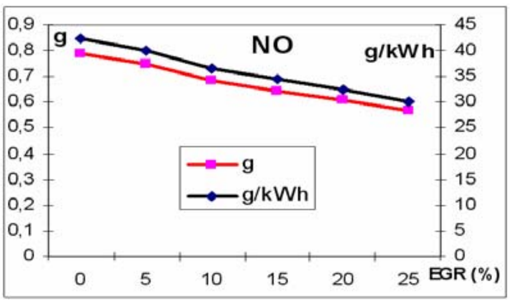
(b) H2O mass evolution



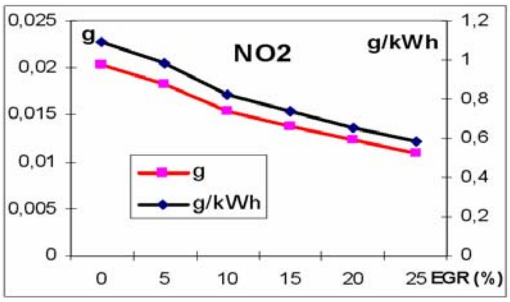
(c) CO2 mass evolution



(d) CO mass evolution



(e) NO mass evolution



(f) NO2 mass evolution

Fig. 8. Evolutions of pollutant emissions in g/cyc/cyl and in g/kWh.

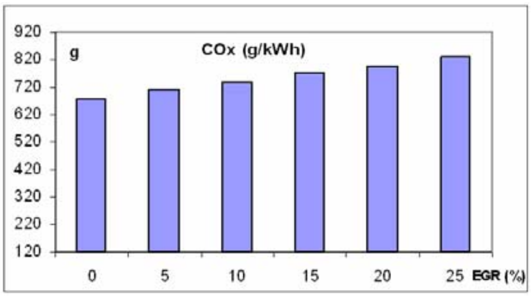


Fig. 9. COx Composition.

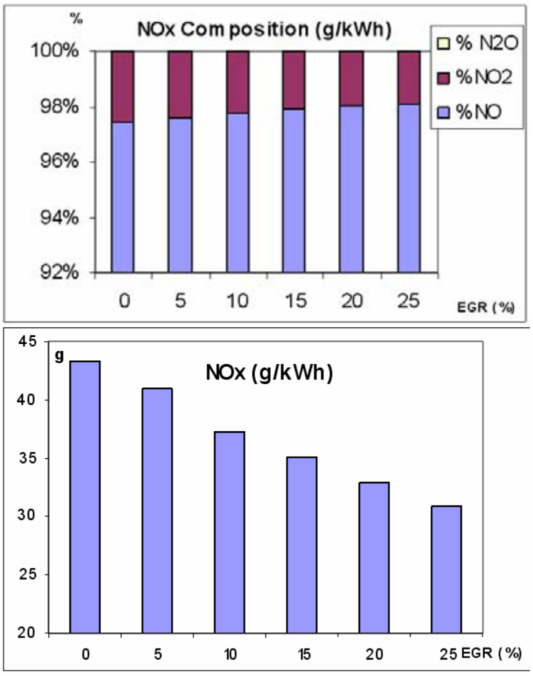


Fig. 10. NOx Composition.

culation on the average combustion temperature, pressure and pollutant emissions along with the various pollutant emissions expressed in g/cyc/cyl and g/kWh .

A considerable decrease in all these parameters is observed. Especially, the NO emission is now way down and can meet the IMO index requirement.

In this case of EGR, the lower oxygen content in “fresh” gas in cylinder admission increases the gas mass brought into play during combustion and consequently the heat-storage capacity, which is also slightly increased by the presence of CO_2 in exhaust gas recycled. Thus, the deficit of oxygen can slow down combustion and shift the cycle towards lower temperature.

This reduction in temperature and in admission air quantity implies a lowering of the NO concentration, which decreases in a quasi linear way according to the rate of exhaust gas recirculation. The fall in the local temperature within the fuel jet also has as a consequence a lengthening of the time of ignition involving a delay of combustion with increase in severity (the quantity of fuel injected during the time undergoing a combustion of mass, is raised).

The level of the fume remains practically constant for a weak rate of exhaust gas recirculation and a quasi linear increase in the CO_2 rate according to the rate of exhaust gas recirculation.

For an average of 10 % in volume of EGR mixed with the admission air, one notes a CO_2 increase on average of 9 % g/kWh; consequently, the emission in COx undergoes an increase, a reduction of NO on average of 12 % g/kWh, and a reduction of NO_2 on average of 21 % g/kWh; consequently, the NOx emission undergoes a reduction on average of 12.3 % g/kWh.

The SOx emission remains constant with EGR .

The exhaust gas recirculation is effective in the reduction in the NOx emissions but requires a sufficient maintenance of the excess of air, under penalty of increasing the consumption and the level of the fume in an important way.

5. Conclusion

To address problems of global air pollution due to the pollutant emission from fuel oil engine combustion, it is necessary to understand the mechanisms by which pollutants are produced in combustion processes. An experimental and numerical study was performed on a unit of real use aboard a car ferry ship. A numerical model based on a detailed chemical kinetics scheme was used to calculate the emissions of CO_2, NO and SO_2 in an internal combustion engine model for the same characteristics of the real unit. In general the experimental and numerical results featured good agreement, especially at high power and for excess air.

For the study of the reduction of pollutant emissions of the diesel engine by the use of exhaust gas recirculation, a substantial decrease in NO was observed, which made the unit meet the IMO regulations.

Nomenclature

A : Preexponential factor
a, b and c : Constants
$C_{..}$: Modeling parameters
C_p : Thermal capacity ($J.Kg^{-1}.K^{-1}$)
$C_{p_{air}}$: Thermal capacity of air ($J.Kg^{-1}.K^{-1}$)
C_{p_g} : Thermal capacity of exhaust gas ($J.Kg^{-1}.K^{-1}$)
D : The engine bore diameter for heat transfer (m)
E_A : Activate energy (J)
EGR : Exhaust gas recirculation
G : Ratio of connecting rod to crank-arm radius
h : heat transfer coefficient ($w.m^{-2}.K^{-1}$)
h_k : Specific enthalpy of the kth species ($J.Kg^{-1}$)
k_f : Forward rate coefficient
$ICEM$: Internal combustion model engine
IMO : International Maritime Organization
$\dot{m}$: Mass flow rate ($Kg.s^{-1}$)
$\overline{M}$: The average molecular mass ($Kg.mol^{-1}$)
MF : Molar fraction
MF_k : Molar fraction of the kth species
M_k : Molar mass of the kth species ($Kg.mol^{-1}$)
m_T : Total mass of the reactants (Kg)
m_{comb} : Mass of the Fuel (Kg)
m_{air} : Mass of the air (Kg)
m_k : Mass of the kth species (Kg)
Nu_h : Nusselt number
P : Pressure (Pa)
P_a : Atmospheric pressure (Pa)
P_{adm} : Admission air pressure (Pa)
P_i : Initial pressure inside the cylinder (Pa)
$P_{motored}$: The motor cylinder pressure (Pa)
P_r : Prandtl number.
PSR : Perfectly stirred reactor
Q : Reactor heat ($J.s^{-1}$)
Q_{wall} : Wall reactor heat loss ($J.s^{-1}$)
r_{air} : Individual gas constant of air ($J.Kg^{-1}.K^{-1}$)
r_g : Individual gas constant of exhaust gas ($J.Kg^{-1}.K^{-1}$)
r_{mix} : Individual gas constant of the mixture ($J.Kg^{-1}.K^{-1}$)
R : Equivalence ratio
R_g : Universal gas constant ($J.kg^{-1}.K^{-1}$)
R_e : Reynolds number
S : The surface area for heat transfer (m^2)
$\overline{S}_p$: Mean piston speed ($m.s^{-1}$)
T : Temperature (K)
T_{air} : Ambient air temperature (K)
T_{adm} : Admission air temperature (K)
T_g : Temperature of exhaust gas (K)
T_i : Initial temperature inside the cylinder (K)
T_m : Exhaust gas temperature (K)
T_{wall} : Chamber wall temperature (K)
V : Reactor volume (m^3)
V_o : Clearance volume (m^3)
V_{air} : Volume of the ambient air (m^3)
V_{cyl} : Volume swept by the piston (m^3)
V_{EGR} : The volume of the recirculate exhaust gas
V_d : Displacement volume (m^3)
V_i : The initial volume inside the cylinder (m^3)
V_m : Exhaust gas volume at the measurement point (m^3)
V_g : Volume of exhaust gas (m^3)
V_{air} : Volume of admission air (m^3)
V_{swirl} : Swirl velocity
Y_k : Mass fraction of the kth species
Z : Gas velocity
Z_{EGR} : Percentage in volume of gas mixed with admission air
λ : Gas conductivity ($w.m^{-1}.K^{-1}$)
λ_a : Air Excess
α : Crank angle (°)
β : Temperature exponent in the rate coefficient
ρ : Density ($Kg.m^{-3}$)
μ : Gas viscosity ($Kg.m^{-1}s^{-1}$)
τ : Residence time in the reactor (s)
$\dot{\omega}_k$: Molar rate of production of the kth species
* : Inlet condition

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