

THE THEORETICAL AND EXPERIMENTAL INVESTIGATION OF THE EFFECT OF VARIATION OF THERMODYNAMICAL PARAMETERS OF EGR FLUID ON NO_x EMISSIONS IN S-I ENGINES

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Abstract Exhaust Gas Recirculation (EGR) concept is the most simple and more economical method for NO pollutant reduction in spark ignition engines. However, when the higher amount of the EGR gas enters into the engine, the power, torque and fuel economy of the engine decrease. One effective solution for reduction of undesirable effect of this method is to use cooled EGR, that results in more reduction of NO pollutant, in the meantime imposing lesser reduction on engine performance. For this purpose a mathematical model has been developed for simulation this method by using two zone combustion model. Results indicate that, when the cooled EGR is used, because of the higher heating specific values of two principle species existed in exhaust gases, namely CO₂ and H₂O, reduction of combustion chamber temperature is higher, hence, the amount of NO emission decreases further. In turn, because of higher specific mass of cooled EGR gas in comparison with hot EGR, the mass of the mixture in cylinder will increase, thus increasing the peak pressure of the combustion chamber accordingly, and so the power output of the engine will not decrease notably in comparison with non EGR case. The comparison shows that there exist good agreement between the experimental and predicted results.

Key Words NO_x Control, Cooled EGR, Spark Ignition Combustion

NO_x pollutant reduction in spark ignition engines. However, when the higher amount of the EGR gas enters into the engine, the power, torque and fuel economy of the engine decrease. One effective solution for reduction of undesirable effect of this method is to use cooled EGR, that results in more reduction of NO pollutant, in the meantime imposing lesser reduction on engine performance. For this purpose a mathematical model has been developed for simulation this method by using two zone combustion model. Results indicate that, when the cooled EGR is used, because of the higher heating specific values of two principle species existed in exhaust gases, namely CO₂ and H₂O, reduction of combustion chamber temperature is higher, hence, the amount of NO emission decreases further. In turn, because of higher specific mass of cooled EGR gas in comparison with hot EGR, the mass of the mixture in cylinder will increase, thus increasing the peak pressure of the combustion chamber accordingly, and so the power output of the engine will not decrease notably in comparison with non EGR case. The comparison shows that there exist good agreement between the experimental and predicted results.

INTRODUCTION

Air pollution caused by the motor vehicles is one the major problems in terms of the environment conservation within any society. three pollutants, namely CO, UHC and NO_x form nearly 98% of the total pollutants [1].

Therefore to limit the amount of pollutants emitted by vehicles, some standards are developed and imposed every year.

Among the gases emitted by SI engines, Nitric oxide (NO), which is colorless and odorless gas, is formed within combustion

chamber and is converted into an exciting nitric dioxide (NO₂) gas in the surrounding atmosphere. The latter one is brownish red in color and odorous. It has been indicated that the toxicity of NO₂ pollutant for human being is nearly five times that of NO and ten times that of CO [2]. Also the NO₂ formed, under sunlight, can interact by unburned hydrocarbons (UHC) existed in the atmosphere producing photochemical smoke which is considered as a secondary pollutant [3]. Moreover NO₂ can interact with the water vapor present in the air to produce nitric acid which has adverse effect on the vegetation.

According to the investigations results and equations available, it is obvious that the concentration of NO pollutant is affected considerably by temperature and oxygen. This means that by controlling these parameters, the concentration of the emitted NO could be reduced. Controlling of NO in SI engines can be done in three ways:

(a) Before introducing of the mixture into the cylinder (i.e. through diluting or pouring the mixture)

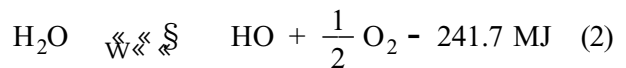
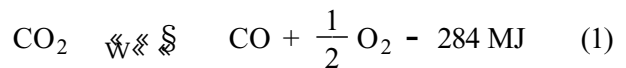
(b) Inside the cylinder through employing of the parameters which affect the propagation and speed of the flame (i.e. imposing some changes on combustion chamber design, creating more turbulent flame, selecting the appropriate ignition system).

(c) After leaving the cylinder, through converting the harmful gases into harmless gases. (i.e. employing catalytic converter).

Considering the solutions given above, the research workers have used variety of methods. It should be mentioned that each one of these methods has its own advantages and disadvantages and it seems that among these methods, the diluting of mixture by exhaust gas recirculation is the most simple and most economical as well as the most suitable method. At part - load condition, when the amount of the EGR is 5 to 10 percent of intake

mixture, the performance of the engine would not be affected considerably [4]. Also it seems that the EGR fluid could improve uneven distribution of the liquid fuel between the cylinders. Figure 1 [5] demonstrates the EGR method schematically in a SI engine. As seen in Figure 1, some of the exhaust gases re-enter to cylinder through an adjustable valve at downstream relative to throttle and mixes with in - coming air - fuel mixture.

The essential effect of EGR on NO formation process pollutant is decreasing of the flame and burned gases temperature due to increase the thermal capacity of the cylinder charge per unit mass of the combustible fuel. Also CO₂ and H₂O which are the most important species in exhaust gases, are dissociated after reaching to flame temperature according to the following equations:



Since the dissociation process is endothermic process, therefore, these gases could absorb part of the heat generated in combustion chamber when they are being dissociated, as a result, decreasing the temperature of gases within combustion chamber further. Moreover when EGR fluid enters the cylinder, the amount of oxygen in the mixture is reduced, so the consequence is dilution of the mixture and reduction in the amount of NO pollutant.

To make the amount of pollutants produced by engines meet the EPA 2004 (Environmental Protection Agency) standards limit, all the possible ways to decrease the amount of pollutants, without having considerable change on engine performance, must be used. It seems that one of the efficient methods to reduce NO pollution is cooled EGR, and in the meantime maintaining the desirable performance of the engine.

Technical literature reveals that there has

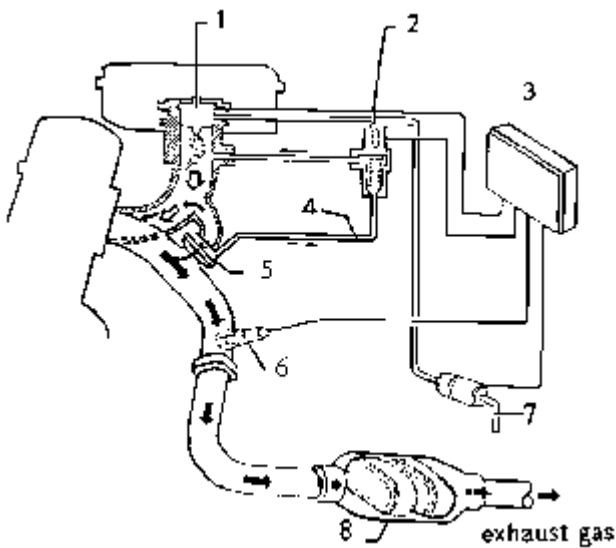


Figure 1. EGR system with catalytic converter on a SI engine: (1) Injection system, (2) Command system of EGR valve, (3) Electronic calculator, (4) Exhaust gas recirculation, (5) EGR valve, (6) Oxygen sonde, (7) Gasoline pump and (8) Catalytic converter.

not yet been any theoretical and experimental work done together on carburetor SI engines with cooled EGR. Therefore in this research work a mathematical model has been constructed to study the effect of thermodynamical parameters of the EGR fluid on NO emission. To validate the theoretical results obtained a carburetor type SI engine has been used.

MECHANISM OF NO FORMATION

Nitric oxide (NO) and nitrogen dioxide (NO₂) are usually grouped together as NO_x emissions where in which, nitric oxide is predominant of nitrogen oxides produced within the engine cylinder. For NO formation three sources can be identified [6].

(a) Nitric oxide which is formed from nitrogen of fuel at reaction zone, and is named fuel NO or chemical NO.

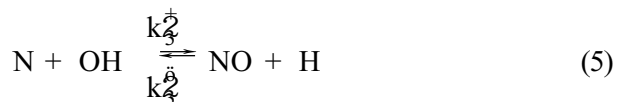
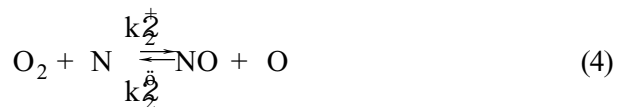
(b) Nitric oxide which is formed exclusively from atmospheric nitrogen inside turbulent

flames of the reaction zone, and is named prompt NO.

(c) Nitric oxide which is produced from atmospheric nitrogen within combustion products and is named thermal NO.

In SöI engines thermal NO is predominant. The amount of nitric oxide in exhaust gases is much more than equilibrium values, hence NO formation reactions are that of rate controlled reactions type. Many mechanisms are proposed in literature for NO formation [6]

In this research work so called extended Zeldovich's mechanism is used and it's reactions explained as follows:



The rate of NO formation via the Reactions 3 to 5 is

$$\frac{d[NO]}{dt} = k_1[O][N_2] - k_2[N][O_2] - k_3[N][OH] + k_2[NO][N] + k_3[NO][O] - k_1[NO][H] \quad (6)$$

where [] denotes concentration of species.

Because the combustion and the NO formation processes are decoupled, it is, therefore, appropriate to approximate the concentrations of O, O₂, OH, H, and N₂ by their equilibrium value at the local pressure and temperature [6].

The following relationship can be used for calculation of rate of NO concentration

$$\frac{d[NO]}{dt} = \frac{2R_1 \left\{ 1 - \left(\frac{[NO]}{[NO]_e} \right)^2 \right\}}{1 + \left(\frac{[NO]}{[NO]_e} \right) R_1 / (R_2 + R_3)} \quad (7)$$

where:

$$R_1 = k_1^- [O]_e [N_2]_e - k_1^- [NO]_e [N]_e$$

$$R_2 = k_2^+ [N]_e [O_2]_e = k_2^- [NO]_e [O]_e$$

$$R_3 = k_3^+ [N]_e [OH]_e = k_3^- [NO]_e [H]_e$$

Where $[]_e$ denote equilibrium concentration of species.

MATHEMATICAL FORMULATION OF THE MODEL

In this work, for calculating thermochemical properties of air-fuel mixture with EGR in a closed cycle, following equations are derived

Assumptions (a) When the EGR fluid mixes with air-fuel mixture, there is't any chemical reaction between them; (b) because of the high velocity of the mixture and short length of the air intake manifold, the fluid transformation within the intake manifold is adiabatic; (c) there is heat transfer between the mixture and cylinder walls during closed cycle of events.

Governing Equations Figure 2 shows pressure-volume diagram of air-fuel cycle. Assuming unsteady flow and the negligible heat transfer between the charge and cylinder walls in the intake process [6], the first law of thermodynamics can be employed:

$$\dot{X}Q + \dot{X}W = dE + dH \quad (8)$$

Assuming $H_e = 0$ (Since no mass can exit from the system's boundary), $E = H - PV$ and $P_i = P_1$, it may be written:

$$H_1 = H_2 + H_i + V_2(P_i - P_e) \quad (9)$$

Assuming $H = nh$, $n_1 = n_{ai-f} + n_{eg} + n_{res}$, $n_{ai-f} = \frac{n_1}{1 + X_{eg} + X_{res}}$, $V_2 = V_{ch}$ and using Equation 9,

the temperature of point 1 (start of compression stroke) can be calculated through

the following relationship:

$$T = \frac{\{(XC_p T)_{res} \cdot X_{ai-f} + (X_{ai-f})[(XC_p T)_{ai} - (XC_p T)_f] - (XC_p T)_f\} - (XC_p T)_{eg} \cdot X_{ai-f} + \frac{V_{ch}}{CP_1} (P_1 - P_e)}{CP_1} \quad (10)$$

$$C_{p1} - X_{ai-f} \left[(XC_p)_{res} + (XC_p)_{ai} - (XC_p)_f - (XC_p)_{eg} \right]$$

$$X_{ai} = \frac{n_{ai}}{n_{ai-1}}, \quad X_f = \frac{n_f}{n_{ai-f}}$$

It is obvious from the Equation 10, that the temperature of the start of compression is affected by the EGR temperature (i.e. T_{eg}). By changing temperature of EGR, T_1 can be changed and as a result the combustion temperature will be changed. So, it is expected to cause reduction of NO formation.

For determination of pressure in the start of compression stroke, it is assumed that:

$$P_1 = P_{ai} + P_f + P_{wa} + P_{eg} \quad (12)$$

Considering that partial pressure of liquid fuel and that of water vapor are negligible, it is possible to apply Equation 13 for determination of pressure at point 1

$$P_1 = P_{ai} + P_{eg} \quad (13)$$

considering Figure 3, that shows EGR fluid circuit in test bed and by assuming that the EGR gas will be in steady state in the surge

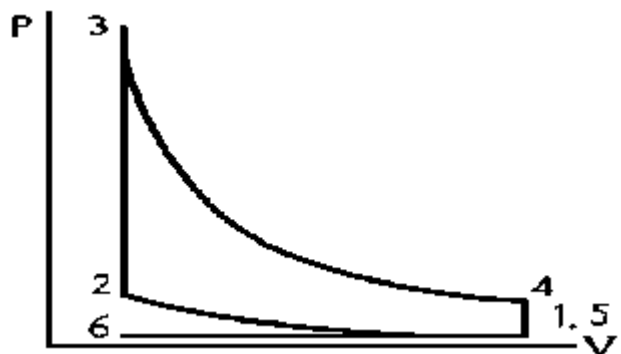


Figure 2. Pressure-volume diagram of constant-volume combustion.

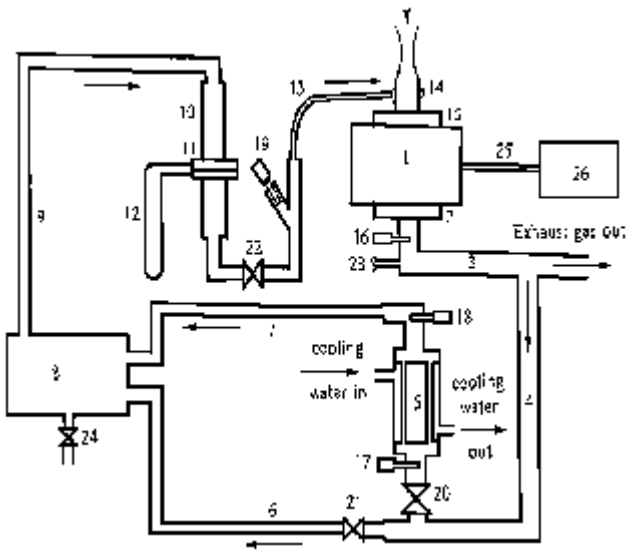


Figure 3. Schematic diagram of EGR circuit: (1) Engine, (2) Exhaust-manifold, (3) Exhaust engine tube, (4) EGR principle tube, (5) Exhaust calorimeter, (6,7) EGR tubes, (8) Surge tank, (9) EGR tube, (10) Flow meter tube, (11) Flow meter, (12) Manometer, (13) EGR copper tube, (14) Spacer, (15) Intake manifold, (16,17,18,19) Thermocouple, (20,21,22) EGR valve, (23) Tube sampling, (24) Surge tank valve, (25) Coupling and (26) Dynamometer.

tank, so the mass, momentum and ideal gas equations can be applied:

$$\dot{m} = f_1 S_1 u_1 = f_2 S_2 u_2 \quad (14)$$

$$S(P_1 \rho_1 u_1 - P_2 \rho_2 u_2) = \dot{m} (u_1 - u_2) \quad (15)$$

$$P = fRT \quad (16)$$

After simultaneous solving of above equations, the specific mass of EGR fluid can be determined from Equation 17

$$y f \rho_2^2 (P_1 z x u_1) \rho_2 x u_1 \rho_1 = 0 \quad (17)$$

where:

$$x = \frac{\dot{m}}{S}, \quad y = RT_2 \quad \text{and} \quad z = \frac{r}{S}$$

Assuming that the wall is isothermal, temperature at the end of step (i.e. T_2) can be calculated from Equation 18

$$\frac{T_w - T_2}{T_w - T_1} = \exp\left(-\frac{hA}{\dot{m}C_p}\right) \quad (18)$$

After determination of f_2 the Equations 14 and 15 can be applied to calculate EGR gas velocity and pressure in EGR outlet tube.

After calculation of the temperature and the pressure at the beginning of the compression stroke (beginning of step), and assuming the cylinder charge being as a closed system, T_2 and P_2 can be obtained at the end of step by applying the first law of thermodynamics (i.e. $\delta Q - \delta W = dF$).

where:

$$F = \sum n_i e_i \quad \text{and} \quad e_i = \sum a_i T^i + e_0$$

a_i is polynomial coefficient, and its value is given in thermodynamics tables [7]. Annand correlation is used for heat transfer calculation between cylinder charge and walls [6]:

$$\frac{q}{A} = a \frac{k}{D} Re^b (T_g - T_w) - c (T_g^4 - T_w^4) \quad (19)$$

where:

$$a = 0.25, \quad b = 0.8, \quad \text{and} \quad c = 3.26 \times 10^{-8}$$

The following equation may be applied for calculation of the work done:

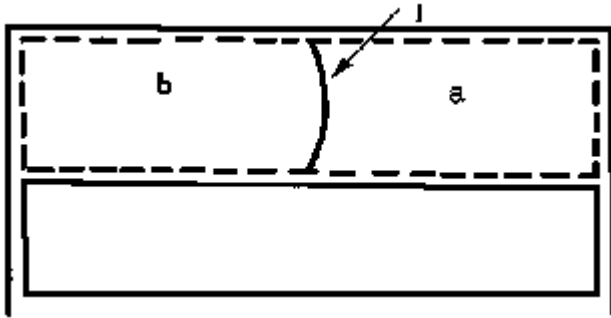
$$\delta W = \int p \, dV \quad (20)$$

After determination of energy equation's parameters and applying numerical methods (i.e. Iteration, Newton-Rafson methods) the temperature and the pressure, can be calculated and as a result, other parameters at the end of the step will be obtained [8]

At the end of the compression process and near the T.D.C. where the mixture have appropriate condition for combustion, the spark plug provides a spark which ignites the mixture and flame front starts up to advance step by step. As a result, cylinder charge will be divided to two zones (Figure 4).

In this research work two zone's model is used for determination of each zone parameters. For calculation of product's temperature (T_b) initial estimate is used as follows [9]

$$T_b = T_u - 2500 \phi (1 - X_{res}) \quad \text{when } \phi \leq 1$$



t= thin flame front, u= unburned gas b= burned gas

Figure 4. Combustion chamber after appearance the flame front.

$$T_b = T'_u \cdot 2500\phi(1 - X_{res}) - 700(\phi - 1)(1 - X_{res})$$

when $\phi > 1$ (21)

from energy balance, the T_b is corrected in such a way that reactant's and product's internal energies shall be equal.

Wiebe function is used here for mass burning rate calculation [10]

$$X_b = 1 - \exp \left\{ -a \left[\frac{\theta - \theta_0}{\Delta\theta_c} \right]^{m+1} \right\}$$

where a and m are adjustable parameters and actual mass fraction burned curves have been fitted with: a=5 and m=2, θ_0 is start of combustion angle, θ is crank angle and $\Delta\theta_c$ is combustion duration (from $X_b=0$ to $X_b=1$).

To establish energy equation, Figure 4 is used and it is assumed that the system boundary is impermeable and flame front which separates two zones from each other is mobile. Unburned mixture is entrained into the flame. In this case the two zones (subsystem) may be compared to two reservoirs, where one of which is filling and the other is emptying. Assuming the process as unsteady, the first law of thermodynamics for each zone will be written as follows:

$$\begin{cases} \delta Q_u + \delta W_u = \frac{dL_u}{dt} + \frac{dL_{tu}}{dt} \\ \delta Q_b + \delta W_b = \frac{dL_b}{dt} + \frac{dL_{tb}}{dt} \end{cases} \quad (23)$$

Considering an uniform-state, uniform - flow

process [11], system of Equations 23 after integration yields to:

$$\begin{cases} Q_u - W_u = E_{u2} - E_{u1} + (m_{u2} - m_{u1})h_u \\ Q_b - W_b = E_{b2} - E_{b1} + (m_{b2} - m_{b1})h_u \end{cases} \quad (24)$$

After solving of the above Equations 24 by numerical method (i.e. Newton), real temperature of each zones will be obtained.

When whole combustible mixture is burned and used by flame, the cylinder contents as combustion products in the case of a single zone model can be calculated. In this state and at each period of time the values of species must be determined via the chemical equilibrium for calculation of the total internal energy of the mixture.

But since generation rate of NO_x is as rate controlled, so for calculation of their amounts, kinetic equations must be applied. Since the values of each species changes in every step, so to calculate the internal energy, the internal energy at zero absolute temperature should be taken in consideration.

RESULTS AND DISCUSSION

In order to calculate combustion parameters and NO emission, the data of a carburetor type, four cylinder, four stroke, 2-valve SI engine is used. It's technical specifications are indicated as below:

cylinder bore	81.5 (mm)
piston stroke	82.5 (mm)
swept volume	1725 (cm ³)
compression ratio	7.5 to 1
nominal power	50 (kW) at 4500 rpm

Also to get the theoretical results, a computer program (in FORTRAN language) for closed cycle with two zones combustion model capable of nitric oxide calculations in kinetic method is written.

To get the experimental results, an hydraulic dynamometer, model Go power (DAö316), for torque measurement, a gas analyser, model

Signal (4000VM), for NO_x measurement based on CLD (chemiluminescence Detector) method, and a gas analyser, model Cussons (P8333), for measurement of CO and UHC emissions based on NDIR, FID methods have been used.

The developed model can predict the amount of NO pollutant with and without EGR at different temperature, at various equivalence ratios under different load/speed conditions.

EGR gas is considered as residual gas which is trapped within the cylinder from previous cycle and its amount depends on pressure difference between exhaust and intake manifolds. Global effect of residual gas is increasing specific heat of the combustion gases, which causes decreasing the peak combustion temperature.

Effect of the EGR temperature on variation of temperature and of the pressure of combustion chamber gases inside the cylinder is shown, theoretically, in reference [12]. There, it has been shown that, by application of cooled EGR, the drop on chamber temperature was high and the drop on pressure was low.

Figure 5 shows NO pollutant variation versus equivalence ratio (Z) obtained from model at $N=2500$ rpm and $\text{EGR}=0$ conditions. The behavior of the curve which is in good agreement with those found in literature [13,14], suggests that the amount of NO pollutant in lean mixture (i.e. $Z=0.95$), has its maximum amount. This is due to high excessive amount of oxygen in lean mixture.

Figure 6 compares the theoretical variation of NO pollutant versus engine speed at full load condition to that of obtained experimentally. As shown in this Figure, firstly, there is a reasonable agreement between the theoretical and experimental findings, and the mean error is about 7%. Secondly, the behavior of both curves which are according to that of observed in literature [15], shows that, when engine speed increases, the amount of NO pollutant

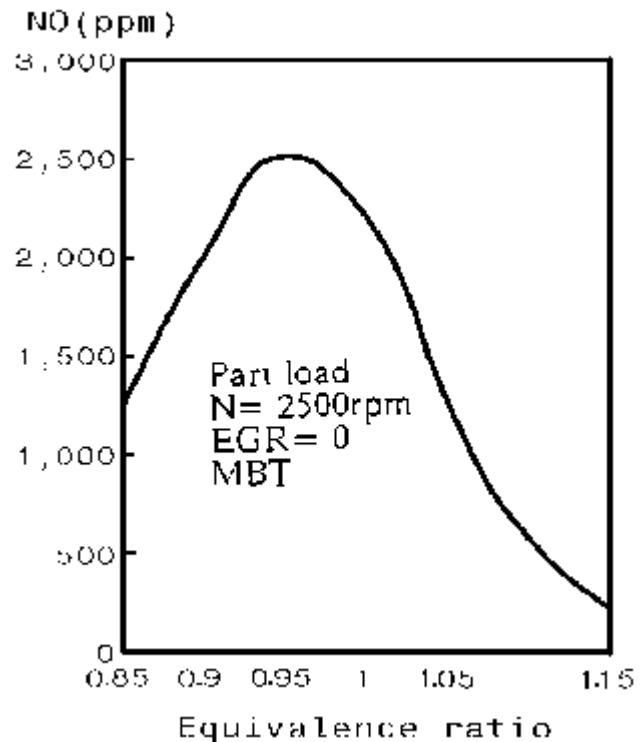


Figure 5. NO pollutant variation versus equivalence ratio.

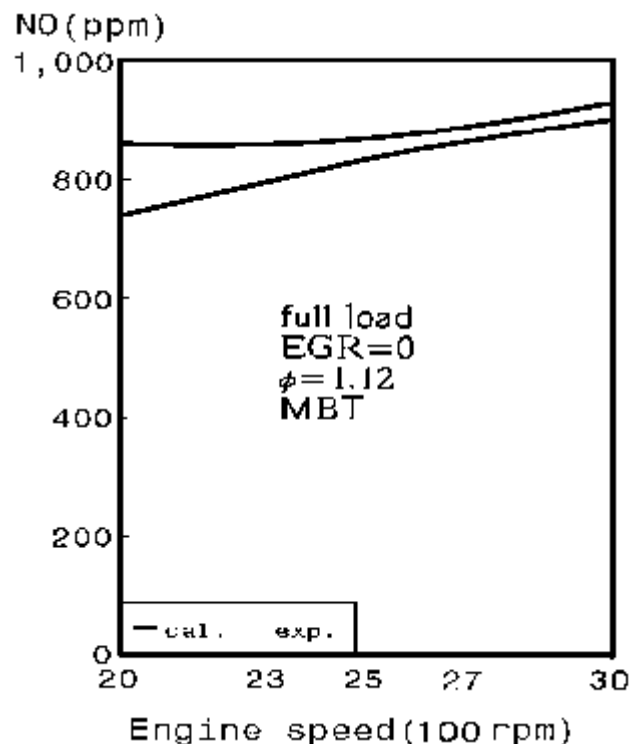


Figure 6. Comparison of the experimental and theoretical pollutant of NO versus engine speed.

increases accordingly. This is due to increase in temperature level which is the main contributor to NO level.

It is evident that better turbulent flow inside combustion chamber due to increasing of engine speed, as well as, decreasing of heat transfer, due to decrease in cycle duration, both contribute to temperature increase.

Generally, at full load condition because the mixture is rich ($Z > 1.1$), the amount of NO pollutant emission is less due to oxygen deficiency.

Comparison of theoretical and experimental results about the effect of quantity as well as the temperature of the EGR on NO pollutant in part load is shown in Figures 7 and 8. As can be seen from the Figure, it is obvious that there is a good agreement between theoretical and the experimental results. Secondly the higher the quantity of EGR and the lower its temperature, drop in quantity of the NO emission will be higher.

Also present model shows that, when EGR fluid with higher temperature is being introduced into the cylinder, the value of the trapped mass decreases, which is in concordance with experimental results [16].

The effect of EGR temperature on engine power that has been obtained experimentally is shown in Figure 9. As shown in this Figure, when a certain amount of EGR (15% in figure) is used at temperature of 350 K, the power loss for the engine would be 6% less than that of the same amount of EGR is used at temperature of 450 K.

Also by increasing EGR quantity, both pressure and temperature of the mixture increase, which are in a perfect concordance with experimental results [17,18], for example, when 10% EGR with 600K is used, the values of temperature and of the pressure increase by 12.7% and 1.17% respectively.

But it is obvious that increasing of pressure causes in decreasing of pumping losses (in P-V

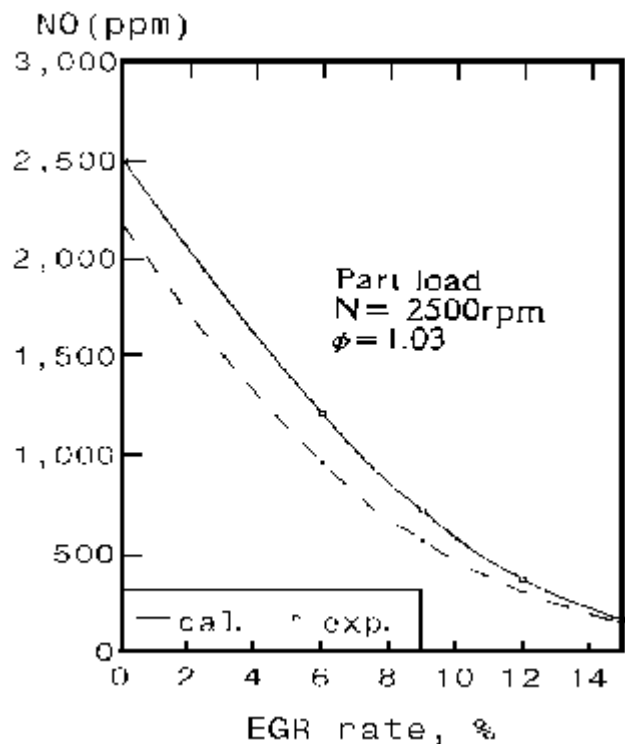


Figure 7. Comparison of the experimental and theoretical effect of the EGR rate on NO emission.

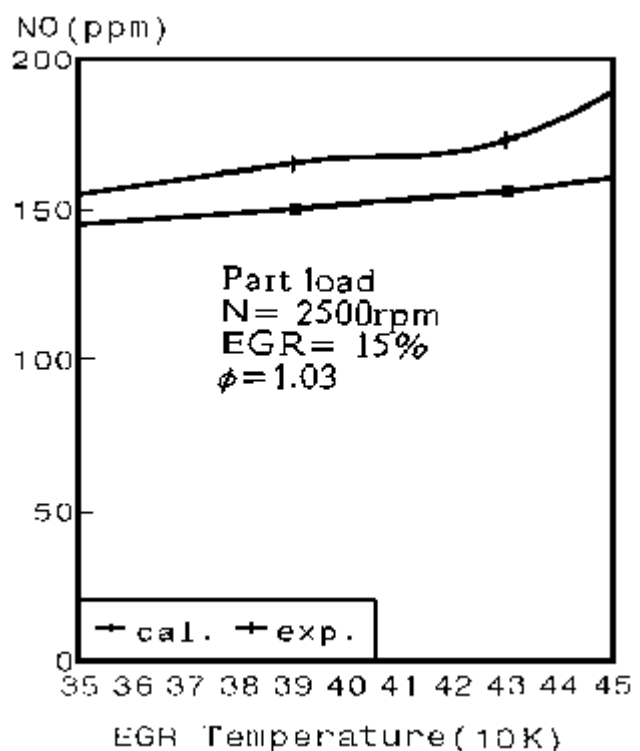


Figure 8. Comparison of the experimental and theoretical effect of the EGR temperature on NO emission.

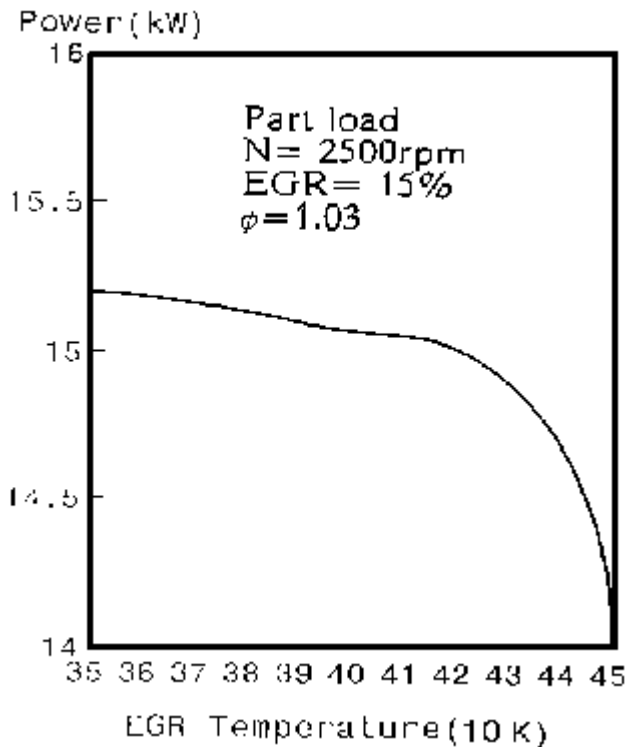


Figure 9. Experimental effect of EGR temperature on engine power.

diagram) and, as a result, indicated work of engine increases. But also in contrary, because of increasing of temperature at the beginning of the compression process, which have more effect on the final temperature of compression process (T_2), increasing of the NO emission occurs.

From the model, it is also seen that, the EGR fluid have a high velocity in carburetor entrance, which have a positive effect on pulverization of the atomized liquid fuel.

CONCLUSION

In this research study, the effect of EGR fluid temperature variations on NO pollutant and other performance parameters on SI engines has been evaluated through mathematical model as well as experimental work. The important results were as follows.

- (1) Among different methods for reduction of NO pollutant, the EGR procedure is the most simple, economical and appropriate.
- (2) The two zone combustion model together

with the EGR and residual gases from the previous cycle can be used in prediction of the thermodynamic parameters (temperature and pressure) which is necessary for calculation of nitrogen oxide.

(3) Beside of NO calculations in the kinetic form, the present model can calculate the equilibrium values of 12 species of exhaust gases at different temperatures

(4) The results of the model constructed on the basis of extended Zeldovich's mechanism used in this research work, had a good agreement in determination of NO pollutant quantity in stoicheometric and also in fairly richer mixtures.

(5) Use of cooled EGR (80°C) in the range of 4 to 9 percent resulted in NO emission reduction by 31% up to 71%, increase in the bsfc by 2.5% up to 3% and also increase in the UHC by 9%.

(6) It is suggested that, in practice, to control the level of NO pollutant, cold EGR to be used instead of hot EGR.

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SYMBOLS

$A(\text{m}^2)$	area
a_i	polynomial coefficient for ith species
$C_p (\text{J/kg.K})$	specific heat at constant pressure
$C_v (\text{J/kg.K})$	specific heat at constant volume
$D(\text{m})$	diameter
$E(\text{J})$	internal energy
$e_i(\text{J/kg})$	specific internal energy for ith species
$e_o(\text{J/kg})$	specific internal energy at zero absolute temperature
$H(\text{J})$	enthalpy
$h (\text{W/m}^2.\text{K})$	convection heat transfer coefficient
$h_i(\text{J/kg})$	specific enthalpy for ith species
$k(\text{W/m}_3.\text{K})$	thermal conductivity coefficient
$k_i^+ (\frac{\text{cm}^3}{\text{mol.s}})$	forward rate constants for ith reaction

$k_i^{\delta} (\frac{\text{cm}^3}{\text{mol.s}})$	backward rate constants for ith reaction
m(kg)	mass
m (kg/s)	mass rate
n	number of moles
P(Pa)	pressure
Q(J)	heat transfer
q (W)	heat transfer rate per unit area
$R (\frac{\text{J}}{\text{kg.K}})$	gas constant
$R_{\text{mol}} (\frac{\text{J}}{\text{mol.K}})$	universal gas constant
Re	Reynolds number
$S(\text{m}^2)$	cross section
T(K)	temperature
u(m/s)	speed
$V(\text{m}^3)$	volume
W(J)	work transfer
X	mole (mass) fraction
$f(\text{kg}/\text{m}^3)$	density
Z	equivalence ratio
h(N)	wall shear force

SUBSCRIPTS

1	start of compression process, beginning of step
2	end of compression process, end of step
ai	air
ai-f	air-fuel
b	burned
ch	combustion chamber
e	exit
eg	EGR
f	fuel
g	gas
i	enter
res	residual
u	unburned
w	wall
wa	water

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