

## Prediction of NO<sub>x</sub> reduction with Exhaust Gas Recirculation using the Flame Temperature Correlation Technique

Arjun Krishnan<sup>1</sup>, Vinay C. Sekar

Mechanical Engineering Department, Indian Institute of Technology Madras

Balaji J, S.M Boopathi

Ashok Leyland Ltd., Hosur, Tamil Nadu

### Abstract:

With emission norms becoming more and more stringent, industries are using technologies like Exhaust Gas Re-circulation (EGR) to reduce NO<sub>x</sub> emissions. This paper discusses a simple methodology for evaluating the effect of EGR on NO<sub>x</sub> reduction based on the Flame Temperature Correlation, which can easily be implemented on a PC. It uses 'base-engine' data to predict by how much NO<sub>x</sub> emissions would reduce for different exhaust gas flow rates, if an EGR system were to be implemented on the engine. The results were compared with experiments and were found to match satisfactorily for industrial purposes for low to medium loads, speeds and EGR flow rates. This method can be used in industries to conduct feasibility studies without performing time consuming and expensive experiments; it can also be used to provide a good set of start values for EGR flow-rate controller optimization.

Keywords: Exhaust gas recirculation, NO<sub>x</sub> control, Diesel engine emissions.

### Introduction

Nitrous Oxides (NO<sub>x</sub> for short) are one of the most harmful pollutants produced by automobiles, damaging the ozone layer and the environment. Hence, countries like U.S, Japan and those in the European Union have come up with more stringent emission norms to reduce the impact on the environment. Serious efforts are being made to reduce the amount of NO<sub>x</sub> emitted by automobiles, especially those using Diesel Engines. There are many techniques available to reduce NO<sub>x</sub>: Retardation of Injection timing, Exhaust Gas Re-circulation (EGR) and Selective Catalytic Reduction (SCR). SCR is the most effective technique, but it is currently difficult to implement on existing cars and trucks due to the extensive modification that must be done to the exhaust system and the prohibitive cost of the technique. Retarding the injection timing reduces engine fuel-efficiency and power output while increasing soot and HC emissions and is hence not favoured. EGR is a cheap and easily implemented option.

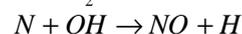
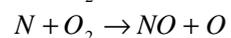
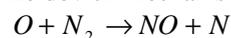
Many people have studied the effects of Intake air dilution using EGR and other gases like N<sub>2</sub> by conducting tests in steady-flow combustors, gas turbines and diesel engines. It has been shown by Ahmad and Plee<sup>1,2</sup> that a strong correlation exists between the stoichiometric-adiabatic flame temperature of the diesel diffusion flame and NO<sub>x</sub> emissions. This has also been confirmed by many other studies.<sup>4</sup>

The purpose of this study was to use this correlation to predict the amount by which EGR will reduce NO<sub>x</sub> emissions, without actually installing an EGR system and conducting experiments. The technique uses only already available, base-engine data like air-fuel ratio, NO<sub>x</sub> emission, etc. for different speeds and loads and predicts what the reduction in NO<sub>x</sub> will be for different rates of EGR flow. This will help the engine manufacturer to estimate quickly whether EGR implementation will serve to reduce NO<sub>x</sub> emissions sufficiently for a particular engine. This procedure may also help in optimizing the EGR-valve control-system quickly by providing it with a set of good start-values for EGR flow rate for different speeds and loads.

### Background and Theory

#### NO<sub>x</sub> FORMATION:

NO<sub>x</sub> (oxides of Nitrogen) formation from atmospheric Nitrogen in any combustor proceeds via the Zeldovich Mechanism.



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<sup>1</sup> Contact email address: arjunkc@iitm.ac.in

Applying the steady state approximation for the  $N_{atom}$  and by assuming that the  $O_{atom}$  is in equilibrium, an equation for the rate of production of  $NO_x$  can be obtained.

$$[NO] \propto [N_2][O_2]^{\frac{1}{2}} e^{\left(\frac{E}{RT_f}\right)} \quad (2)$$

$E$  = Activation energy for the reaction (kJ/kg)

$R$  = Universal Gas Constant, (kJ/kg.K)

As indicated by this equation, the  $NO$  production is a strong function of temperature and is not influenced by Oxygen and Nitrogen concentrations much. Indeed, studies on Steady-Flow combustors (by Bowman first) also corroborate this fact.

#### DIESEL COMBUSTION:

It is well established that the Diesel Combustion process consists of three-stages:

- Ignition Delay phase: where no combustion takes place and the diesel spray evaporates and mixes with air.
- Pre-mixed burning stage: where this pre-mixed diesel ignites and burns. Since this fuel is already pre-mixed, the rate of combustion is controlled entirely by chemical kinetics
- Diffusion burning: where the majority of the injected diesel burns. The diesel spray evaporates and mixes with air and then burns. The mixing of Diesel and air here is rate-controlling.<sup>3</sup>

It was also shown by Lyn<sup>3</sup> that the most amount of energy is released during the diffusion burning phase. Hence, fuel packets which burn during this phase reach the highest temperatures and the most amount of  $NO_x$  is formed here.

#### FLAME TEMPERATURE CORRELATION:

Several investigators have used the characteristics of simple-diffusion flames to model diesel combustion and  $NO_x$  production in the diesel engine. Sawyer et al. argued that  $NO_x$  emissions from Diesel engines should correlate with the adiabatic flame temperature just like in gas turbines and other steady-flow combustors. Since most of the diesel burns in the diffusion burning phase and  $NO_x$  forms primarily in the burned-gas region, we can assume that most of the diesel burns in the diffusion phase. Hence, the adiabatic-stoichiometric Flame Temperature calculated at SoC should correlate well with  $NO_x$  emissions. Indeed, this has been shown by Plee<sup>1,2</sup> to be true and  $NO_x$  produced can be described using an equation of the form:

$$EI_{NO_x} = C_{mix} e^{\left(\frac{-38700}{T_f}\right)} \quad ; \text{ With } E/R = -38700K \quad (3)$$

$C_{mix}$  = mixing factor dependant on speed and load but not on intake composition (dilution or EGR). See Fig. 1

$EI_{NO_x}$  = Emission Index.  $NO_x$  in grams/ kg of fuel

$T_f$  = Calculated Adiabatic-stoichiometric flame temperature at start-of-combustion

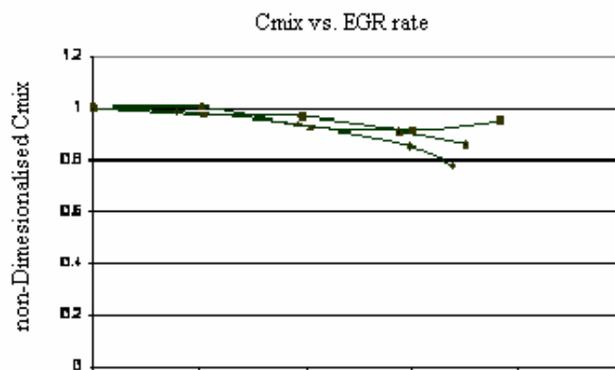


Fig 1  $C_{mix}$  vs EGR flow-rate

In Fig.1, the variation of the  $C_{mix}$  factor with EGR flow rate at three different engine operating conditions is shown. Actual experimental values are used for  $EINO_x$  at different EGR rates, and the flame temperature is calculated using our software. This must be verified by actually measuring adiabatic flame temperature using techniques available in literature instead of calculating it. But this graph is sufficient for illustration and justification of the assumptions.

Yu and Shahed<sup>4</sup> have confirmed these results for IDI and DI-Diesel engines. They also showed that calculating  $T_f$  at TDC does not affect the correlation coefficient much. We know that the fuel packets which burn

first reach the highest temperatures and it follows that the most NOx must form in these packets. Start-of-combustion in diesel engines is usually a few degrees before TDC and these few degrees do not make much difference. This study uses this correlation technique to predict NOx levels, with modest but sufficient accuracy (90%) if EGR is implemented in an engine for different exhaust-gas flow-rates. Given base-engine data like air-flow, fuel-flow, speed, load and NOx emissions, we can predict the reduction in NOx levels on implementation of an EGR system.

## Experimental Setup and Experiments

The engine details have been given in Table 1 and the block diagram is given in Fig 2.

Table 1. Engine Specifications

Engine type	6 cylinder, inline
Power	14.8 kW/ litre@2400rpm
Torque	68.3Nm/ litre@1400rpm
Fuelling	Direct Injection, inline pump
Turbocharger	Single stage, intercooled

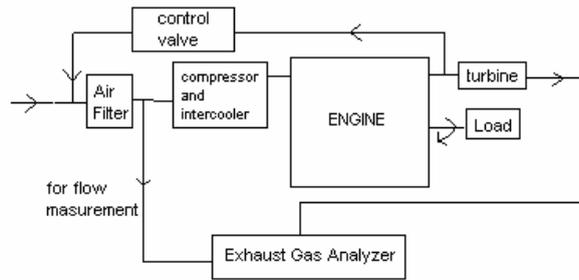


Fig 2 Experimental Setup Block Diagram

The Engine was first tested at different speeds and loads. Fuel flow rate was measured using a coriolis-effect mass-flow meter. NOx and CO<sub>2</sub> levels were measured with a chemiluminescent analyzer (CLA) and a Non-dispersive infrared analyzer (NDIR) respectively. Bosch smoke numbers were also recorded. The EGR system was then installed and exhaust was fed in before the air-filter. This was to avoid fouling of the intercooler, cylinder and compressor blades. On an engine in which EGR is implemented, the wear effects of EGR must be combated separately by using more corrosion resistant materials and low-sulphur fuel. Exhaust gas flow-rates were measured by comparing CO<sub>2</sub> concentrations in the exhaust gas and intake air. Then the EGR mole fraction  $x$ , is expressed as:

$$x = \frac{N_{CO_2, intake} - N_{CO_2, reference}}{N_{CO_2, exhaust} - N_{CO_2, reference}} \quad (4)$$

Where N represents number of moles. The gas and location where the number of moles is measured is given in the subscript.

Experiments were conducted for EGR flow rates at various speeds and loads and emissions were obtained and compared with the theoretical calculation.

## Predicting NOx levels with EGR

### THE EFFECTS OF EGR:

The addition of Exhaust-Gas has many effects on diesel engine combustion and pollutant formation.

They are:

1. Decreased flame temperature due to increased heat capacity of the intake charge<sup>7</sup>.
2. Lower O<sub>2</sub> concentration due to dilution of the intake charge. Exhaust gas contains much lower O<sub>2</sub> levels than ambient air.
3. Increasing the inlet temperature due to introduction of hot combustion products
4. Changes in Ignition Delay and combustion characteristics like flame structure
5. Increased inlet concentration of pollutants due to re-circulation, leading mainly to greater in-cylinder wear-rates.
6. 'Thermal throttling' effect: the hot exhaust-gases mix with cooler air in the intake manifold. This reduces the density of the intake mixture and hence the mass of the inducted charge decreases. This causes an overall increase in cylinder temperatures.<sup>6</sup>

### CALCULATING FLAME TEMPERATURE:

The parameters required for calculating flame temperature are the number of moles undergoing combustion, volume, temperature and pressure at Start of Combustion (SoC) and the composition of the gas (concentrations of various species). The angle at which the second derivative of the Cylinder Pressure vs. crank angle (P vs.  $\theta$ ) curve goes through a minimum is taken as SoC. The minimum is considered between -10 and +10 degrees, with TDC taken as 0 degrees.

To find gas parameters at SoC, we need to know the intake charge composition and its temperature and pressure at the beginning of the compression stroke. The number of moles of gas inducted can be obtained from the air flow-rate, boost pressure and temperature in the intake manifold. Volume of the intake charge, once the intake valve closes a little after the piston passes BDC is nearly equal to the engine displacement volume. Temperature and pressure calculations are described in the next section. The gas parameters (temperature, pressure, etc.) must be obtained at SoC. It is sufficient to assume that the charge undergoes an isentropic (adiabatic-reversible) process since the variation in  $C_p$  with temperature ( $< 1000K$ ) does not affect the calculation. Other effects like heat-loss through cylinder walls are do not have a great effect on flame-temperature. Hence,

$$P_o V_o^g = P V^g \quad (5)$$

Once all the parameters of the gas at Start-of-Combustion are obtained, we can calculate the adiabatic-stoichiometric flame temperature. The energy equation for adiabatic combustion at constant pressure is:

$$(H_{products}(T_f) - H_{products}(T_{298K})) - (H_{reactants}(T_o) - H_{reactants}(T_{298K})) = Q_{cv} \quad (6)$$

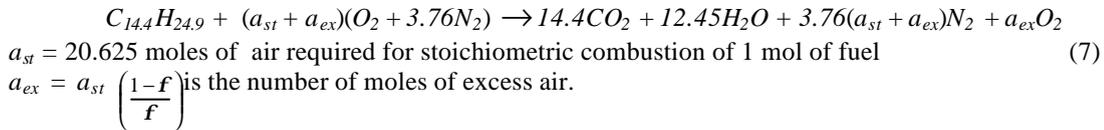
$Q_{cv}$  = Calorific value of diesel at NTP  
 $H$  = Enthalpy of products\reactants  
 $T_o$  = Temperature at SoC

We must solve this equation using the Newton-Raphson technique: the flame temperature must be guessed and we must see if the energy equation is satisfied.

#### MODELLING:

It has been shown<sup>1,2,6</sup> that the most important effect of EGR on NOx formation is the increased heat capacity. In other words, the flame temperature changes significantly only due the change in heat capacity. The flame temperature is to be calculated taking into consideration only the change in heat capacity due to re-circulation of polyatomic CO<sub>2</sub> and H<sub>2</sub>O. The effect of decreased O<sub>2</sub> levels on combustion characteristics like ignition delay, burn rate and heat-release is ignored.

The chemical equation describing Diesel combustion, when there is no dilution, is:

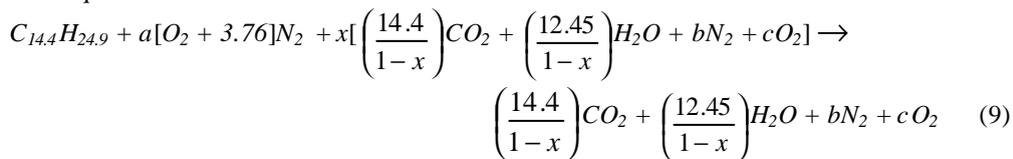


F is the equivalence ratio

On addition of EGR, a complex, feedback-like process takes place. Since pollutants are constantly being fed back into the cylinder, it can be expected that the pollutant concentration will continuously increase. But experiments have shown that this is not the case, and CO<sub>2</sub>, H<sub>2</sub>O and emissions reach a constant steady-state value. This can also be 'proved' theoretically. It can be shown that if the EGR flow rate is x (moles of exhaust gas re-circulated / net moles of exhaust), the CO<sub>2</sub>, H<sub>2</sub>O and pollutant concentrations converge like a geometric sequence to steady-state concentrations. This is contrary to intuition, which says that as more and more CO<sub>2</sub> and H<sub>2</sub>O are re-circulated, the concentrations in the cylinder must continuously increase.

$$\begin{aligned} \text{Moles of CO}_2/\text{mol of fuel} &= 14.4(x + x^2 + x^3 + \dots) = \left( \frac{14.4x}{1-x} \right) \\ \text{Moles of H}_2\text{O}/\text{mol of fuel} &= 12.45(x + x^2 + x^3 + \dots) = \left( \frac{12.45x}{1-x} \right) \end{aligned} \quad (8)$$

The chemical equation for combustion on addition of EGR becomes:



where,  $b = \frac{3.76a}{1-x}$  and  $c = \frac{a - a_{st}}{1-x}$  can be obtained using chemical species balance.

#### Thermal Throttling:

This effect is significant on the NOx reduction properties of Exhaust Gas re-circulation. It increases the temperature of the intake charge and thereby reduces density. This causes a decrease in the heat-capacity of the charge and hence there is an overall increase in cylinder temperatures. Consider the control volume, which is shown in Fig 3.

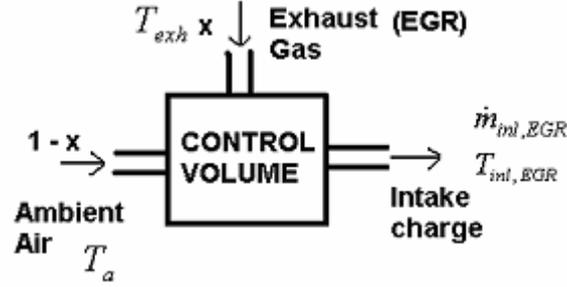


Fig 3 Control volume at point where exhaust mixes with intake

Density of an ideal gas  $\rho \propto \frac{1}{T}$  Mass flow rate of air =  $\dot{m} = \rho \dot{V}$  Hence,  $\frac{\dot{m}_{inl,EGR}}{\dot{m}_{inl,base}} = \frac{T_{inl,base}}{T_{inl,EGR}}$  (9)

The engine volumetric efficiency is the same for the given speed and load. Hence, the number of moles of gas inducted per cycle is calculated as follows

$$\eta_{volumetric} = \frac{V_{inducted,EGR}}{V_{displaced}} = \frac{V_{inducted,base}}{V_{displaced}} \quad n_{moles,EGR} = \frac{P_{inl,EGR} V_{inl,EGR}}{RT_{inl,EGR}} \quad (10)$$

Applying the steady flow energy equation to this adiabatic control volume, we get:

$$\dot{m}_{a,EGR} h_{a,EGR} + \dot{m}_{EGR} h_{EGR} = \dot{m}_{inl,EGR} h_{inl,EGR}$$

$\dot{m}_{a,EGR}$  = mass flow rate of ambient air

$\dot{m}_{EGR}$  = mass flow rate of EGR through the EGR pipeline

$\dot{m}_{inl,EGR}$  = mass flow rate of inlet charge to the engine

$$\text{Hence, } (1-x)\bar{h}_a + x\bar{h}_{exh,EGR} = \bar{h}_{inl,EGR} \quad (11)$$

where  $h_{EGR}$ ,  $h_{a,EGR}$ ,  $h_{inl,EGR}$  corresponding specific enthalpies

The ambient air and exhaust gas enthalpies are known since we know their temperature and composition. The only thing left to calculate is the temperature of the mixed charge, the 'Mixing temperature'. This again can be solved by guessing mixing temperatures, calculating enthalpies and checking whether equation (11) is satisfied.

*Inlet manifold pressure (boost pressure):*

The boost pressure (after inter-cooler), or  $P_{inl,EGR}$  according to our convention, changes when EGR is added because of the change in mass-flow rate through the turbocharger. For a compressor with constant inlet conditions and similarly for a turbine, the equations are:

$$\dot{W}_{comp} \propto \dot{m}_{comp,base} \left[ \left( \frac{P_{boost}}{P_{inlet}} \right)^{\frac{g-1}{g}} - 1 \right] \quad \dot{W}_{turb} \propto \dot{m}_{turb,base} \left[ 1 - \left( \frac{P_2}{P_1} \right)^{\frac{g-1}{g}} \right] \quad (12)$$

These mass-flows can be written as:

$$\dot{m}_{comp,base} = \dot{m}_{a,base} \dot{m}_{comp,EGR} = (1-x_m)\dot{m}_{inl,EGR}$$

$$\dot{m}_{turbinebase} = \dot{m}_{a,base} + \dot{m}_{fuel} \dot{m}_{turbine,EGR} = (1-x_m)\dot{m}_{inl,EGR} + \dot{m}_{fuel} \quad (13)$$

where  $x_m$  the EGR mass ratio is given by  $x_m = \frac{x \times M_{wt,EGR}}{M_{wt,inl,EGR}}$

With the following assumptions the new boost pressure equation can be formulated:

- Exhaust Temperature remains the same after EGR introduction. Reasons as detailed in above section
- Exhaust backpressure and pressure drop across turbine remain the same.

- The mass flow rate of fuel for both engines is to be maintained constant. This is, in fact, the assumption we made to normalize the flame temperature correlation.

#### *Pressure at start of compression stroke ( $P_{BDC}$ ):*

The pressure at the inlet manifold is known and since we know the mass-flow rate of charge, we know the volume that fills the cylinder at inlet manifold conditions of pressure and temperature. Assuming an adiabatic process, we may calculate the pressure at BDC since the volume of the cylinder is known.

#### *Exhaust Gas temperature:*

1. Combustion rate is slower due to lowered  $O_2$  concentration and hence combustion continues much later into the expansion stroke than usual, causing an increase in the exhaust gas temperature.
2. The increased heat capacity due to inclusion of polyatomic  $CO_2$  and  $H_2O$  reduces temperatures reached by the gas.
3. Inclusion of hot exhaust gases in the intake charge increases exhaust gas temperature

The exhaust temperature remains un-affected because of the above three effects being in balance. It has also been shown by Ladomattos (*et al.*)<sup>6, 7</sup> that exhaust gas temperature is affected to a very small degree through EGR addition. The exhaust gas temperature can also be solved for by considering heat and mass balance for the entire engine, but this complicates the equations and hence has not been incorporated at this juncture.

#### *Ignition Delay:*

It has not been shown by experiment that the change in ignition delay due to EGR or dilution does not significantly affect flame temperature. But, a simple calculation using the observed ignition delay in an engine with EGR reveals that the change in adiabatic-stoichiometric flame temperature is very small: the change in predicted  $NO_x$  values changes by only 0.2% with a large ( $5^\circ$ ) change in Ignition delay. So this effect is ignored. We just calculate the flame temperature using TDC as our reference point.<sup>2</sup>

#### STEP-BY-STEP PROCEDURE ADOPTED TO CALCULATE EINO<sub>x</sub>

1. Obtain Base-Engine data for various speeds and loads. The required parameters to be measured for each speed and load are:
  - a. Air flow-rate (kg / hr)
  - b. Fuel flow-rate (kg/hr)
  - c.  $NO_x$  emissions (ppm)
  - d. Temperature, Intake manifold (K)
  - e. Temperature, Exhaust (K)
  - f. Pressure, Intake manifold (bar)
  - g. Cylinder Pressure vs. Crank Angle data
2. Estimate Exhaust Temperature
 

If Hot (Un-cooled) EGR is used, the exhaust temperature for the base engine is assumed as the exhaust temperature for the engine even when EGR is applied. If a Cooler is employed (Cooled-EGR), then we must estimate the temperature of the exhaust gas before it is fed into the system. We can either use the temperature to which we would want to cool the exhaust gas, or assume typical heat-exchanger efficiencies and calculate the temperature of the exhaust gas.

This turns out to be useful: We can now use different exhaust-gas temperatures and find out how much the  $NO_x$  reduction is, and design the heat-exchanger accordingly. But there are other effects of cooling the exhaust gas: soot emissions and combustion efficiencies have been found to increase. These effects must also be taken into consideration when designing the EGR cooler.
3. Estimate EGR engine data:
  - a. Assuming an EGR flow-rate, the chemical composition of the charge can be calculated.
  - b. The mixing temperature and mass-flow rate are determined.
  - c. The manifold pressure for the EGR engine is calculated.
  - d. Pressure, volume and temperature at BDC can now be calculated.
  - e. Using ideal-gas isentropic compression relations, all the parameters at SoC are obtained.
4. Flame temperature calculation: As detailed above

Once all these parameters are obtained, the flame temperature can be calculated using equation (6).

## Results and Analysis

The EINO<sub>x</sub> values were normalized with base-engine values and the graphs for different loads at 2400rpm and 100% load at different speeds were plotted. It is clear from Fig 4 and 5 that the correlation between

theoretical and experimental values is very good for low EGR rates. This is obvious: for low levels of dilution, combustion characteristics like ignition delay and burn-rate are unaffected and so is the intake manifold temperature. The only significant effect is that of the increased heat capacity of Inlet charge due to incorporation of CO<sub>2</sub> and H<sub>2</sub>O. As the amount of exhaust gas dilution increases, other effects, notably those on combustion, become increasingly significant.

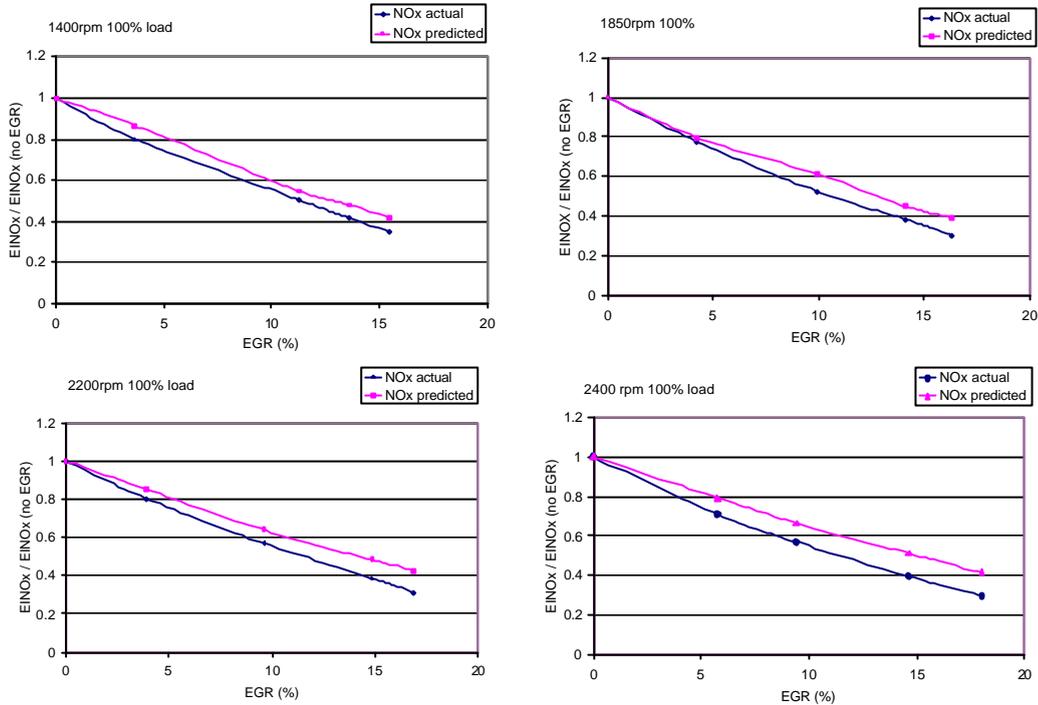


Fig. 4 EINOx vs EGR Rate (%) 100% Load, Different Speeds

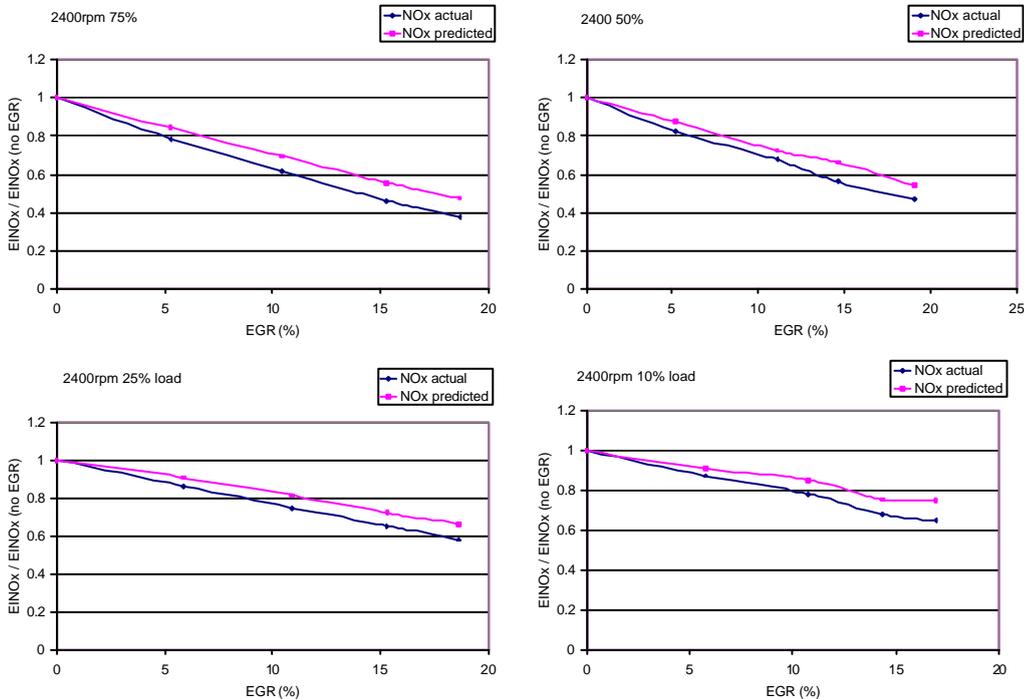


Fig. 5 EINOx vs EGR Rate (%) 2400rpm (Max. Power speed), Different Loads

It is also clear that the greatest divergence from predicted values is at high loads and speeds (See graphs for 75 and 100% load at 2400 rpm in Fig 4). At high loads, the air-fuel ratio is close to stoichiometric and hence lesser oxygen is available. This available O<sub>2</sub> is further decreased due to exhaust gas dilution. Burn rates and heat at these conditions are affected significantly and hence so is NOx production.

The software consistently predicts higher values of NO<sub>x</sub> emission at all conditions. This is useful at the design stage since it gives an upper-bound figure for NO<sub>x</sub> reduction (least possible decrease). The reasons for this will be analysed in detail at a later stage.

Nevertheless, the correlation, on the whole, is very good and the accuracy is sufficient for industrial purposes. The averaged errors over speed and load over a range of EGR flow rates (in %) are shown in Fig. 5. The graphs show increasing error with EGR rate, as expected. The highest errors are at high speed and load conditions due to the aforementioned reasons: At 100% load the average error over a range of speeds is 17.6 %, which is on the higher side. At lower loads (25%), the errors fall considerably and the average error over all EGR flow rates and speeds is about 6.5%.

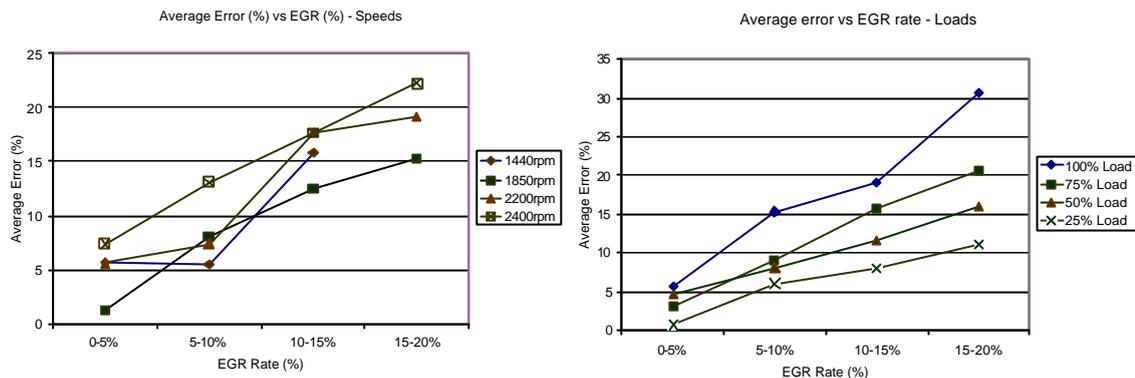


Fig. 6 Averaged errors (speed, load) vs. EGR Rate (%)

## Conclusions

A procedure was developed to calculate the reduction in NO<sub>x</sub> levels due to EGR, given only engine base-data. This approach utilised the flame temperature correlation technique to obtain NO<sub>x</sub> predictions with sufficient accuracy – 6.5% at low loads. The correlation coefficient was also high for medium-to-low load conditions. This procedure can be adopted for industrial purposes and feasibility studies on EGR. It can also be used to optimize EGR-Valve controllers by providing it with a set of good start values. Errors are significant at 100% load condition and high EGR rates at all speeds. We think that a more accurate calculation of flame temperature, by inclusion of CO<sub>2</sub> dissociation and other effects, will improve the results. This analysis will be conducted in future studies. Standard equilibrium temperature calculation software like the NASA package can also be used instead of the simple procedure outlined here.

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