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Numerical Prediction of NO_X in the Exhaust of a Compression Ignition Engine

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***Abstract*—**For numerical prediction of the NO_X in the exhaust of a compression ignition engine a model was developed by considering the parameter equivalence ratio. This model was validated by comparing the predicted results of NO_X with experimental ones. The ultimate aim of the work was to access the applicability, robustness and performance of the improved NO_X model against other NO_X models.

***Keywords*—**Biodiesel fueled engine, equivalence ratio, Compression ignition engine, exhausts gas temperature, NO_X formation.

I. Introduction

THE nitrogen oxides produced during combustion have been heavily investigated for over two decades. Many techniques have been developed to prevent the formation of NO_X within the combustion chambers of the engine (primary action) and to reduce the already formed NO_X within the exhaust gases (secondary action).The operational condition of diesel engines like high pressure, high temperature and heterogeneous charge are particularly challenging for the current NO_X models.

It is well known that *NOx* emissions are related to start of combustion timing and the energy released in premixed burning. Earlier start of combustion causes higher cylinder pressure and higher combustion temperature, which cause higher *NOx* emissions. More energy released in premixed combustion causes more rapid cylinder pressure rise and higher combustion temperatures that consequently elevate *NOx* emissions. The spray cone angle also elevates the *NOx* in biodiesel fuelled vehicles.

The higher surface tension and viscosity of biodiesel fuels could reduce spray angle, and the earlier combustion could also suppress the spray cone formed. It was also observed that start of injection of biodiesel fuels was earlier than that of diesel fuel, which also had a significant effect on *NOx* emissions.

From literature four applicable procedures for adjusting NO_X emission levels for ambient temperatures & humidity were available. For heavy duty vehicles the relationship includes effects of both temperature and humidity referenced to standard conditions of 29.4^0 C and 10.71 g/kg of humidity. The K for KNO_X indicates that the NO_X values have been corrected for humidity. The humidity factor ranges from 0.88 to 1.05.Following equation was based upon the work by Krause, et al., [1].

$$KNO_X = 1 + A\,(H-75) + B\,(T-85)$$

Where:

$A = 0.004\,(F/A) - 0.0038$

$B = -0.116(F/A) + 0.0053$

where F/A is the fuel to air ratio by mass.

Krause, et al., [1] in his further study also presented more generalized equation considering ambient temperatures & humidity without the F/A term.

$$KNO_X = 1 - 0.00216(H-75) + 0.00076\,(T-85)$$

The effects of temperature and humidity on light-duty diesel engines were investigated by Hare and Bradow [2]. The test was conducted on four naturally aspirated diesel engines. The resulting correction for ambient conditions included only humidity effects, as the range of temperature variation was very small.

$$KNO_X = 1 - 0.0152\,(H-10.71)$$

In order to predict numerically, the percentage of NO_X in the exhaust of compression engine, the authors have incorporated the emission model based on the equivalence ratio. In present study the combustion model for compression ignition engine was investigated. Then, the NO_X formation process in the engine was analyzed.

In the compression ignition engine, the emission process is numerically analyzed and the validity of this model was examined according to experimental results referred. Consequently, this model can calculate the emission under actual engine operating conditions. By using the experimental results, the relation between equivalence ratio and NO_X emission were identified and then by using Newton's forward difference method the model was developed.

II. Emission Factors: NO_X & Equivalence Ratio

A. Developed Model

Emission factor for *NOx* are generally measured, however can be calculated based on the equivalence ratio ϕ. The present model uses equivalence ratio to compute *NOx* emissions directly as shown below,

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$$NOx = \frac{c\phi}{\left[23.47 - 73.45\phi + 70.15\phi^2 - 18.37\phi^3\right]}$$

(Where value of C ranges in between 1 & 4)

Where NO_X is in gm/kw-hr. The above expression was initially derived on the assumption that NO_X emission is directly proportional to equivalence ratio.

Definition of Equivalence Ratio used:

$$\phi = \left[\frac{m_f}{m_a}\right]_{act} / \left[\frac{m_f}{m_a}\right]_{st}$$

B. Approach and Assumptions in NO_X Model

The developed model considers single zone approach. The important assumption made in the model is NO_X as a function of local temperature & equivalence ratio. The basic purpose of the model is to predict and calculate the NO_X based on the equivalence ratio.

C. The Goal of Emission Compliance

The goal of emission compliance further restricts the design possibilities for an optimized I.C. engine. In order to eliminate the production of NO_X, the fuel/air mixture must be homogeneous and very lean at the time of combustion. When preparing for the NO_X formation models need a calibration procedure to match the predicted data with the experimental data.

Although the calibration methods are different with each model, burned gas temperature is used to calibrate with its calculated data. But, considering the degree of dependency of NO_X formation on temperature, it would be hard to admit that this calibrated burned gas temperature is appropriate for NO_X modeling. Therefore in present modeling, the equivalence ratio was selected.

III. Engine Specifications

Following are technical specifications of the engine on which the tests were performed and results were used for developing the NO_X model.

TABLE I
TECHNICAL ENGINE SPECIFICATIONS

No of cylinders	4
Max Power	66kw@ 4200 RPM
Max Speed	4800 RPM
Compression Ratio	19:1

IV. Results & Discussions

The experimental NO_X emissions with change in equivalence ratio, exhaust gas temperature with change in RPM, equivalence ratio with exhaust gas temperature & RPM at every state were obtained and graphs were plotted. In this study, experiments were performed on a four-cylinder, four-stroke, and diesel-engine. The basic specifications of the engine are shown in Table I. These results were used as reference to develop the actual models. The results used as reference were taken from Openshaw K, et al. [14], Srivastava A, et al. [15] and Krause, et al. [1].

A. Trend in Changes in Oxides of Nitrogen Emission with Variation in Equivalence Ratio

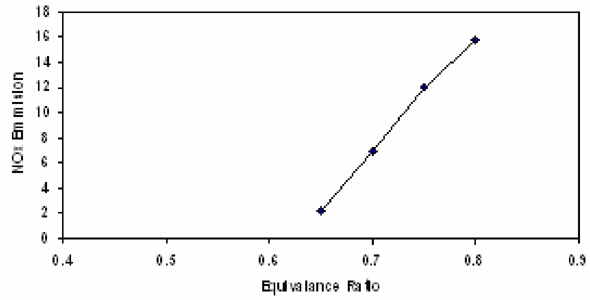

Fig. 1 Equivalence ratio Vs NO_X Emission

From Fig. 1, it is observed that the average increase of NO_X emission (gm/kw-hr) with increase in equivalence ratio & biodiesel is 206%, it may be due to the oxygen percentage available in the mixture is more as the mixture is lean i.e. Φ‹ 1 where Φ is equivalence ratio.

B. Difference in Experimental NO_x & Calculated NO_x

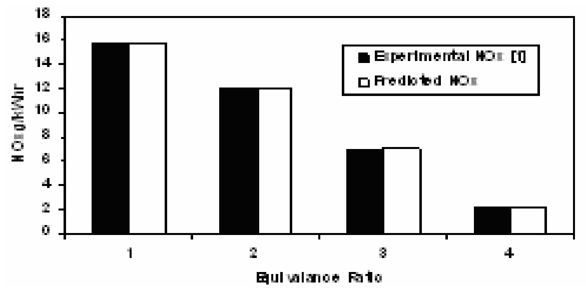

Fig. 2 Experimental NO_X vs. predicted NO_X

From Fig. 2, it is clearly understood that there is very slight variation in the values of predicted & calculated NOX emission. The maximum difference of 0.19% occurs at Φ = 0.8 (1) and minimum difference of 0% occurs at Φ = 0.75 (2) in between predicted and calculated NOX values.

C. Trend in Changes of Exhaust Gas Temperature with RPM

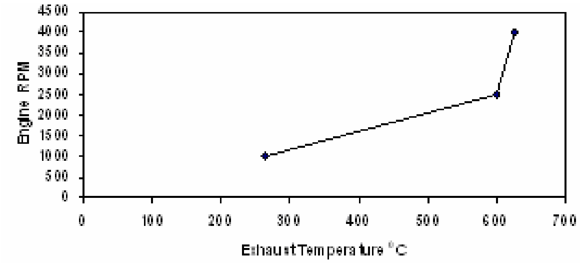

Fig. 3 Exhaust gas Temperature Vs Engine RPM

From Fig. 3, it is clearly understood that as the engine speed increases the exhaust gas temperature increases and this relationship also depends upon the engine load. At ¼ load and when engine speed is 1000 RPM the minimum temperature of 262 ^{0}C is achieved and maximum temperature of 626.3 ^{0}C is achieved at ¾ load.

D. Trend in Changes of Equivalence Ratio with Exhaust Gas Temperature

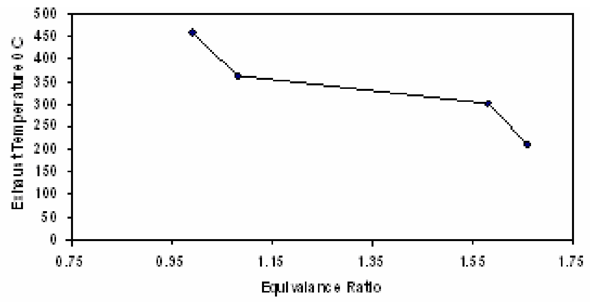

Fig. 4 Equivalence Ratio Vs Exhaust Temperature

From Fig. 4, it is clearly understood that maximum temperature is achieved when mixture is lean i.e. when Φ is below 1 and minimum temperature is achieved when Φ is above 1.

E. Trend in Changes of Correction Factor with RPM

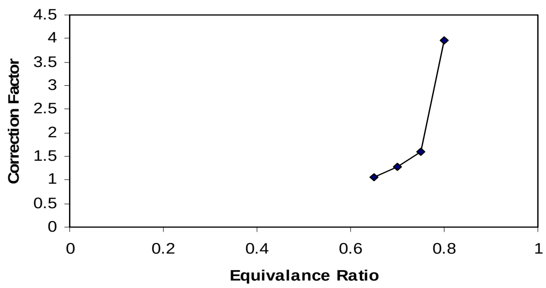

Fig. 5 Correction Factor Vs Equivalence Ratio

F. Comparison of Predicted and Measured NO_X Emissions

Biodiesel	**Equivalence Ratio ϕ**			
	0.65	**0.70**	**0.75**	**0.80**
Measured NO_X (g/kw-h)	**2.2**	**7**	**12**	**15.75**
Predicted $NO_{X(g/kw\text{-}h)}$	**2.201**	**7.0114**	**12**	**15.721**
Relative Error	**0.184**	**0.16**	**0**	**0.045**

The correction factor for Φ=0.65, C=1.056, for Φ=0.70, C=1.028, Φ=0.65, C=1.6 and for Φ=0.65, C=3.95.

V. CONCLUSION

In this study, a numerical emission model for predicting the NO_X formation has been investigated.

As a result, it has been shown that the authors model have been enabled the numerical predictions of the behavior of NOX formation along with the equivalence ratio in the multicylinder compression ignition engine. Comparison of the calculated results of the NOX formation in the I.C.engine with the experimental results has been revealed the following. The model can be used for Multicylinder biodiesel fueled diesel engines and maybe used for single cylinder biodiesel fueled diesel engines.

The value of Φ as it increases the NOX increases and maximum error occurs at Φ =0.65 and minimum error occurs at Φ =0.75. The experimental and calculated results generally show very similar trends. However a further improvement of model is required for the evaluation of NO_X emission when equivalence ratio become rich.

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