REDUCING DIESEL ENGINE EMISSIONS

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ABSTRACT

Diesel engine exhaust emission constituents, particularly oxides of nitrogen (NO_x) and Particulate Matter (PM), have potentially wide-ranging detrimental effects on ecosystems, buildings and human health. Their control will be critical in order to alleviate the future pressures on the global environment. Many diesel emission control strategies have been implemented over the last twenty years, with the result that the emissions levels from diesel passenger vehicles have been reduced by 80-90%. However, there is still much work to do in order to meet the proposed EU and US-EPA legislative limits.

One of the factors currently limiting the effectiveness of exhaust emissions reduction technologies arises from the relatively poor transient response characteristics of existing on-board exhaust gas NO_x sensors. This limits their use in feedback control strategies. The work described here illustrates one possible method of overcoming this limitation, using an indirect approach. This is based on measurement of instantaneous cylinder pressure–volume data, in combination with simplified models for in-cylinder NO_x and PM formation. These models are based on fundamentals of chemistry and thermodynamics but employ some empiricism in order to minimise computational time. Results to date are encouraging and it is envisaged that the method could find application in low emissions diesel engines of the future.

INTRODUCTION

The world is facing a serious environmental dilemma. Since the 1950s, its population has more than doubled and the global economy has grown nearly six-fold. The automotive industry has also grown rapidly, with worldwide production increasing from 8.1 million units p.a. in the 1950's to 35.6 million units p.a. in the 1980's. More recently, European throughout has increased from 14.33 million units in 1995 to 17.21 million units in 2001 [1]. Diesel engine automobile production has also undergone strong growth and the market share in Europe for diesel-engined passenger cars rose from 32% in 2000 to over 40% in 2002. Austria, Belgium and France all showed a passenger car market share of over 60% for diesels in 2002, with all 15 countries of Western Europe showing an increased diesel passenger car market share since 1990.

Diesel engines emit less CO_2 per energy output than any other IC engine, with levels up to 20% lower than their gasoline counterparts [2]. Current levels of carbon monoxide (CO) and unburned hydrocarbon (HC) emissions from diesels are not significant when compared to spark ignition engines [3]. Since the levels of these pollutants are low they do not require post-combustion treatment in order to comply with emissions regulations and so are of minor importance.

Oxides of nitrogen (NO_x) and Particulate Matter (PM) emitted from diesel combustion systems have been identified as having wide-ranging detrimental effects on ecosystems, buildings and human health [4] and their control will be critical in the future success of the diesel engine. Figure 1 illustrates the progressive decreases in maximum permitted levels of emission from heavy duty diesel engines in Europe.

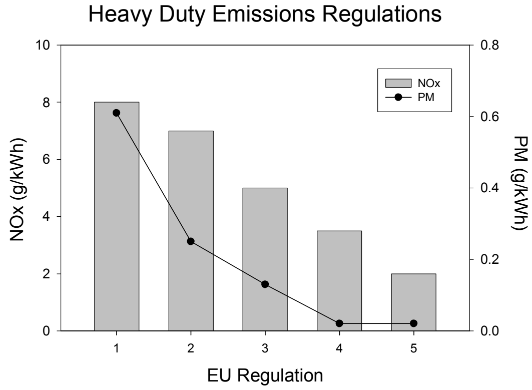


Figure 1: European Legislative Limits for Heavy Duty Diesel NO_x and Particulate Matter

THERMODYNAMIC MODELLING OF DIESEL CMBUSTION PROCESSES

The last century has seen engineers and researchers intensify their theoretical end experimental efforts to improve diesel combustion systems by lowering emissions whilst maintaining low fuel consumption. Simple theoretical approaches are based on the First Law of Thermodynamics [5]. These so-called zero-dimensional models assume uniformity of the composition and temperature of the in-cylinder mixture and assume that the fuel injected instantaneously mixes with a mixture of ideal, in-cylinder gases. Advancement on these models requires details of the local physics of combustion and aim at prediction of the time dependent mixture formation and rate of heat release in discrete volumes [6,7]. This discretisation of the combustion chamber allows for a more realistic description of the temperature and composition inhomogeneity within the cylinder but a limitation of these multiple zone models is that extrapolation to different engines is difficult, and so a generic multi-zone model has to date not been identified. Also, as the number of model zones increases so too does the computational time.

Some of the most detailed approaches to engine modelling are based on Computational Fluid Dynamics (CFD). The equations of conservation of mass, momentum and energy are all incorporated into this type of model [8] and these allow for the simulation of individual processes in both the time and space domains. The combustion chamber is divided into many discrete volumes – possibly as many as 40,000 elements. This leads to long computational times, which in turn renders these models unsuitable for practical real-time application in the automotive industry.

The present study explores a simplified, semi-empirical approach to analysis of measured cylinder pressure-volume data. This aims to capture the evolution of relevant physical and chemical data over the combustion cycle and to subsequently quantify rates of pollutant formation. Taking this information together with those parameters measured in engine testing known to affect NO_x and soot formation, realistic prediction schemes with relatively few empirical constants have been developed. Computational time is kept low and good quality predictions are obtained, leading to the possibility of this method being used in a real-time automotive onboard system.

NO_x MODELLING

The parameters incorporated into the NO_x estimation scheme were those known to greatly influence NO_x formation: namely the rate of fuel mass burned (RFMB), adiabatic flame temperatures and the chemistry of NO_x formation. These factors were determined using simplified calculations stemming from measured in-cylinder pressure and a zero-dimensional thermodynamic model [9].

The following equation was developed to estimate the number of kmol of nitric oxide formed in the burnt volume ΔVb during the time step associated with one crank interval (0.5^o crank).

$$(eNOx) = \frac{1}{6.n.NSTEP} \sum_{CAD=SOD}^{EOC} \frac{R_u \cdot T_{ad}}{P \cdot MW_b} \cdot \Delta FMB.\frac{Const.}{T^{1/2}} \cdot \exp\left(\frac{-Ea}{T}\right) \cdot [N_2]_e \cdot [O_2]_e^{0.5} \cdot \Delta CAD \qquad (1)$$

P is the instantaneous cylinder pressure T is local temperature at which the NO_x formation occurs, T_{ad} is the adiabatic flame temperature, Ea is the activation energy, and $[N_2]_e$ and $[O_2]_e$ represent the equilibrium concentrations of nitrogen and oxygen respectively in a mixture of gases which are dissociated at high temperatures. *NSTEP* is the number of calculation steps performed per crank angle degree (*CAD*) and *ΔFMB* is the incremental fraction of fuel mass burned during the calculation step. n is the engine speed.

In order to facilitate direct comparison with the experimental INO_x, the estimated NO_x variable (eNO_x) was transformed into specific units (grams of NOx emitted per kg of fuel injected) and is denoted *IeNOx*.

Various empirical relationships were investigated to identify empirical constants which could be used, along with the theoretical formulations above, to "*predict*" or "*estimate*" NO_x levels from the in-cylinder data so that this could be compared with the actual NO_x levels recorded from the engine exhaust stream. It is accepted that Equation (1) will not yield correct magnitudes and statistical tools were introduced at this stage, in combination with substantial quantities of experimental data, in order to determine the empirical constants and to assess the capability of the model to reproduce trends. Following trials with numerous formulations, the expression given as Equation (2) was found to be satisfactory:

$$ln(INO_x) = A + B \cdot ln(Fr) + C \cdot ln(n) + D \cdot ln(IeNOx) + E \cdot (ln(n))^2 + F \cdot (ln(IeNOx))^2 \qquad (2)$$

This equates the natural logarithm of the measured NO_x emission index INO_x (measured mass in *grams* of NOx emitted per *kg* of fuel injected) to a function which includes six empirical constants (A through F). Variable n is the engine speed (rev.min^{-1}) and Fr is the fuel/air equivalence ratio. A total of 521 test cases were used to establish the model constants. Light Duty and Heavy Duty test cases were treated separately.

MODELLING OF SOOT FORMATION

The soot found in the exhaust stream of the diesel engine was estimated from measured P-V data, using a form of the two-stage Hiroyasu model [10]. Although the exact mechanisms of soot formation and oxidation in diesel combustion chambers are not fully understood, it is established that temperature, pressure and equivalence ratio each have an effect. The soot formation and oxidation rates are described by equations (3) and (4) respectively;

$$\frac{dm_{sf}}{dt} = A_f \cdot Fuel_m \cdot P^{0.5} \cdot e^{-\left(E_f / R_u T\right)} \tag{3}$$

$$\frac{dm_{so}}{dt} = A_o \cdot Soot_{net} \cdot \left(\frac{P_{O_2}}{P}\right) \cdot P^{1.8} \cdot e^{-\left(E_o / R_u T\right)} \tag{4}$$

The values of E_f and E_o were taken from the literature [11, 12] at 52,300 KJ/kmol and 58,576 KJ/kmol, respectively. Soot oxidation is continuously occurring and hence must be taken into consideration in calculation of the net soot amount exhausted, (5).

$$\frac{dm_s}{dt} = \frac{dm_{sf}}{dt} - \frac{dm_{so}}{dt} \tag{5}$$

dm_s / dt is then integrated to give the emissions index *IeSoot* (in units of *grams* of soot exhausted per *kg* of fuel injected).

Based on these equations, a soot prediction methodology was derived using a procedure broadly similar to that used for NO_x estimation. Equation (6) employs a number of empirical constants (A^* through F^*) in order to generate values of *ISoot*, the soot emission index (in grams of soot per kg of fuel injected).

$$ISoot = A^* + B^* IeSoot + C^*.Fr + D^*.n + E^*.Fr^2 + F^*.n^2 \tag{6}$$

The soot model was verified using data from one light duty engine covering a wide range of operating conditions.

STATISTICAL ADJUSTMENT

The constants needed in the semi-empirical equations (Equations (2) and (6)) for estimation or "prediction" of NO_x and Soot levels were identified using statistical software (Statgraphics Plus 5). This involved adjusting the free variables (A through F and A^* through F^*) to achieve best fit between the "estimated" and the experimental values. Regressions were performed employing a Taylor series model. The optimum values obtained for the constants (*A* through *F*) in the NO_x analysis are given in Table 1, for the Light and Heavy Duty engine cases respectively.

Engine	A	B	C	D	E	F
Light Duty	79.12	-0.93	9.5	8.99	-0.67	0.18
Heavy Duty	105.9	-0.57	6.69	10.41	-0.47	0.21

Table 1: Optimum values for the constants obtained in solving Equation (3) – NO_x model.

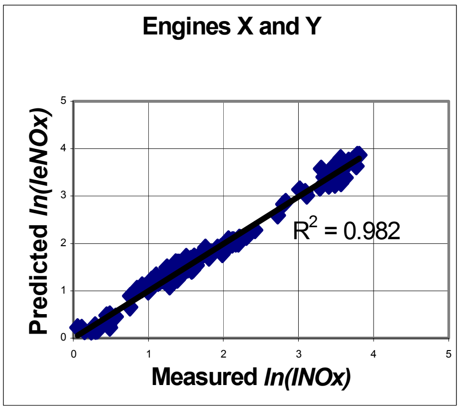
Equation (6) was applied to data from Light Duty engine testing to identify the soot model constants given in Table 2. These were based on 116 test cases, carried out over a wide range of engine operating conditions.

Engine	A^*	B^*	C^*	D^*	E^*	F^*
Light Duty	7.99	-7.79×10^{-4}	-33.81	-0.0028	59.36	1.06×10^{-6}

Table 2: Showing the values for the constants obtained for Equation (7) – Soot model.

Verification of the quality of the "*predicted*" versus measured values of lNO_x and *lSoot* was undertaken using a variety of statistical techniques. Good applicability was found.

The application of equation (2) to NO_x estimation for engines X and Y gives an adjusted correlation coefficient R^2 value of 0.982, (Figure 2). This highlights the applicability of this regression methodology to Light Duty engine test cases.



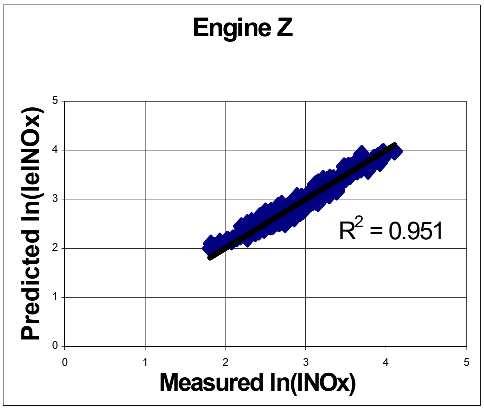


Figure 2: "*Predicted*" versus measured specific NOx emissions for (a) Light Duty Engines X and Y (log scales) and (b) for Heavy Duty Engine Z (log scales)

Similar trends also evident in the results of soot estimation for the Heavy Duty engine cases (Figure 2 (b)), with an adjusted R^2 value of 0.951 being achieved.

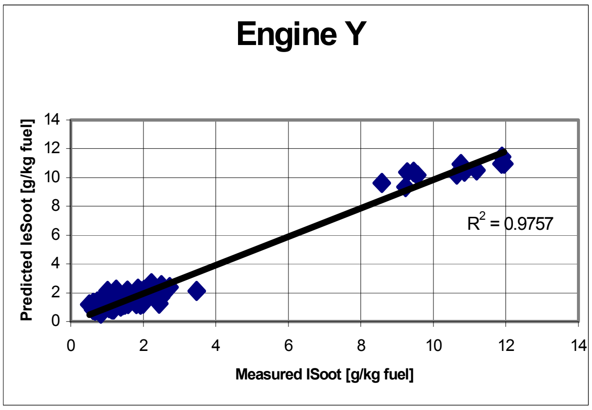


Figure 3: "*Predicted*" versus measured specific soot emissions for Light Duty engine Y.

These very satisfactory trend predictions were repeated in the soot prediction model, as illustrated in Figure 3. Note that this graph uses linear scales and that an adjusted R^2 value of 0.976 was achieved. Again this gives a clear indication of the success of the semi-empirical model "*predictions*" in matching the experimentally measured soot values.

CONCLUSIONS

This study describes the development and verification of semi-empirical calculation schemes that use modelling methods to "*predict*" the NO_x and soot concentrations found in the exhaust stream of a compression ignition combustion engine. The objective was to develop methods of rapidly estimating pollutant quantities produced during each engine cycle, based on input of measured P-V data.

The model developed tracks the evolution of physical and chemical parameters that are known to have a strong influence on the formation of NO_x and soot emissions. A number of major simplifying assumptions have been implemented to ensure that the computation time is kept to a minimum. These do not appear to have seriously compromised the quality of the final results but the NO_x calculation scheme currently relies on separate sets of empirical constants for Light and Heavy duty engines.

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