

Phenomenological Modelling of Oxygen-Enriched Combustion and Pollutant Formation in Heavy-Duty Diesel Engines using Exhaust Gas Recirculation

Dimitrios Hountalas and Spiridon Raptotasios
National Technical Univ. of Athens

Theodoros Zannis
Hellenic Naval Academy

Roussos Papagiannakis
Hellenic Air Force Academy

ABSTRACT

A theoretical study is conducted to examine the effects of oxygen enrichment of intake air and exhaust gas recirculation (EGR) on heavy-duty (HD) diesel engine performance characteristics and pollutant emissions. A phenomenological multi-zone model was properly modified and used to assess the impact of intake air oxygen-enhancement and EGR on the operating and environmental behavior of a HD diesel engine under various operating conditions. Initially, an experimental validation was performed to assess the predictive ability of the multi-zone model using existing data from a HD turbocharged common-rail diesel engine at the 12 operating points of the European Stationary Cycle (ESC) considering certain high-pressure cooled EGR rate at each operating point. A theoretical investigation was conducted for diesel operation without EGR considering a variation of intake air oxygen fraction from 21% to 25%v/v under the following two operating modes: (1) Constant fuelling rate and (2) Increased fuelling rate to sustain constant in-cylinder average air/fuel equivalence ratio (λ). The predictions of this analysis showed a considerable reduction of exhaust soot and small improvement of brake specific fuel consumption (BSFC). However, in both modes of oxygen-enhanced diesel operation, a significant increase of NO emissions was observed, which created the motivation to examine the implementation of EGR. Hence, a second theoretical investigation was performed considering variation of high-pressure cooled EGR from 0% to 30%v/v for the aforementioned intake air oxygen mole fractions under two different modes of engine operation: (1) Constant inlet pressure and (2) Increased inlet pressure to sustain constant average air/fuel equivalence ratio (λ). The theoretical results of this combined analysis showed a considerable reduction of soot and NO emissions accompanied by limited or imperceptible penalties in BSFC, which are more pronounced in the case of constant λ due to increase of brake power output. Consequently, there is a promising path for simultaneous reduction of soot and NO emissions from heavy-duty diesel engines without serious detrimental effects on specific fuel consumption by combining intake air oxygen-enrichment and cooled EGR.

CITATION: Hountalas, D., Raptotasios, S., Zannis, T. and Papagiannakis, R., "Phenomenological Modelling of Oxygen-Enriched Combustion and Pollutant Formation in Heavy-Duty Diesel Engines using Exhaust Gas Recirculation," *SAE Int. J. Engines* 5(4):2012, doi:10.4271/2012-01-1725.

INTRODUCTION

During recent decades, research has endeavored to increase power and thermal efficiency, while suppressing gaseous and particulate emissions of pollutants of diesel engines to comply with increasingly stringent environmental regulations. An effective method to improve combustion

effectiveness and to reduce emissions of particulates (soot) from diesel engines is the enhancement of incylinder oxygen availability [1]. This can be done by either mixing diesel oil with oxygenated additives or by increasing the oxygen concentration in the cylinder intake air [1,2,3,4]. According to previous studies [1,2,3,4,5,6,7,8,9], the increase of intake oxygen mole concentration results in increase of peak

cylinder pressure, reduction of ignition delay and drastic reduction of particulate emissions, CO and unburned hydrocarbons. Specifically, Karim and Ward [10] studied the effect of the partial pressure of oxygen (up to 50%) in the intake charge of a DI diesel engine and noticed large reductions in ignition delay and smoke emissions. Cylinder pressure increased with oxygen concentration, whereas the rate of pressure rise reached a maximum at about 38% oxygen and then leveled out. In addition, Ghojel *et al.* [11] studied oxygen enrichment of the intake charge of an IDI diesel engine. Increasing the intake oxygen mole fraction from 21% to 40 % led to a large decrease in ignition delay and reduced combustion noise. Also, the experiments of Ghojel *et al.* [11] showed that HC and CO emissions decreased, and smoke levels dropped drastically, whereas NOx emissions increased commensurately with the oxygen added. Most important, this study [11] showed that the increase of intake oxygen content from 21% to 25%v/v at high fuelling rates may result in an increase of indicated power output up to 10%. Similar observations concerning reduction of HC, CO and smoke emissions, shortening of ignition delay and increase of NOx emissions with increasing supply air oxygen percentage were made by Iida and Sato [12] and Iida *et al.* [13]. In addition, Watson *et al.* [14] studied oxygen enrichment of the intake air, up to 30%, in two direct injection (DI) diesel engines and reported 80% reduction of particulate emissions at full load. They reported the opportunity for achieving engine outputs comparable to those of turbo-charged engines, with consequential benefits of increased power/mass ratios. Hence, they recommended the substitution of the engine turbocharger and inter-cooling system with a smaller turbocharger and polymeric membrane elements to supply the oxygen-enriched stream. This would have dual benefits as the smaller turbocharger would have improved transient response and the smaller induction system would be lighter and less costly. As a drawback they reported an increase of NOx by a factor of 2, which increase however, could be curtailed to 50% by retarding the injection timing.

The practical viability of intake air oxygen-enrichment has been hampered by the slow pace of developing compact and inexpensive on-board devices that extract oxygen from air [15,16,17,18]. In recent years, progress has been made in the development of compact, high productivity air separation membranes, such as highly selective polymeric membranes. According to Nemser *et al.* [18], modern hollow fiber membranes employed for either oxygen-enrichment of intake air operate at substantially lower pressure differentials and much higher volumetric gas rates than those applied for industrial nitrogen generation. In addition, this type of membranes offers low pressure loss in the oxygen-enrichment stream, moderate pressure ratios across the hollow fiber wall, compact size for incorporation in the intake air system, good transient response and they are robust, lightweight and suited to engine operating environment [18].

Studies conducted in the past have proposed various techniques such as diluent addition (CO_2 , N_2 and EGR) in engine supply charge and retardation of injection timing for controlling NOx emissions [19,20,21,22,23]. Specifically, Desai *et al.* [19] stated that the deterioration of NOx emissions may be controlled by selecting an optimum combination of intake air oxygen percentage and fuel injection timing. Virk *et al.* [22] limited oxygen enrichment of intake air to 21.5 and 22.5% and retarded the fuel injection timing to avoid such large increases in NOx emissions. By doing so, they managed to reduce particulate emissions by 15-30% while maintaining same levels of NOx emissions with conventional diesel operation. The study of Virk *et al.* [22] revealed that injection process manipulation seems to be promising towards attenuating NOx emissions without exacerbating soot emissions in cases intake air is oxygen-enriched. This way the NOx after-treatment system that will be used to further minimize NOx emissions will be less demanding. The necessity for an optimum combination of oxygen fraction in intake air with a NOx reduction technique was also acknowledged by Byun *et al.* [23]. They conducted tests in a single-cylinder and a six-cylinder diesel engine using gas separation membranes in order to attain various oxygen concentrations in the supply air. They concluded that the smoke density of both engines was remarkably reduced (35-73%) due to oxygen-enriched diesel combustion.

Tsunemoto and Ishitani [24] as well as Yu and Shahed [25] investigated the diluents' addition (EGR, CO_2 and N_2) in conjunction with intake air oxygenation. Their results showed that gas dilution is effective in reducing NO emissions at the expense of increasing smoke. Carbon dioxide proved to be most effective diluent in reducing NO emissions, followed by EGR and nitrogen respectively. In addition, Perez and Boehman [26] attempted to specify the optimum operational conditions for oxygen-enriched combustion in a single-cylinder DI diesel engine in order to reduce PM emissions with minimal exacerbation of NOx emissions by controlling fuel injection timing, CO_2 and O_2 volume fractions in intake air. They reported that at the condition of 23%v/v O_2 and 10%v/v CO_2 , NOx emissions were reduced by 46% with respect to baseline operation [26]. They concluded that smoke emissions in diesel engines can seriously be reduced with no essential negative effects on NOx emissions when oxygen-enriched intake-air is mixed with CO_2 [26]. However, most of the experimental studies conducted in the past with intake oxygen-enrichment and gaseous diluents focused on experimental single-cylinder diesel engines with conventional low-pressure fuel injection systems [24,25,26,27]. Hence, the relative changes observed in engine performance parameters and exhaust emissions from the application of intake air oxygenation and diluent addition cannot be extrapolated to other types of diesel engines and especially, to commercial heavy-duty (HD) diesel engines with electronic high-pressure fuel injection systems. In addition, it has not been shown by up to what extent is

possible to moderate the negative effect of oxygen enrichment on NO_x emissions using EGR in common-rail heavy-duty diesel engines without dampening the positive effects of oxygen enrichment on power enhancement and on decreasing exhaust soot.

Hence, a theoretical study is performed to investigate the effects of intake air oxygen-enrichment and exhaust gas recirculation (EGR) on heavy-duty (HD) diesel engine performance and pollutant emissions. A multi-zone model was properly modified and used to evaluate the influence of intake air oxygen content and EGR rate on the operational and environmental behavior of a HD diesel engine under various operating points. The predictive ability of the engine simulation model was assessed against existing experimental data from a HD common-rail diesel engine at the 12 operating points (3 engine speeds and 4 loads) of the European Stationary Cycle (ESC) considering certain rate of high-pressure cooled EGR at each operating condition. Initially, a parametric study was performed to examine the impact of intake air oxygen content from 21% to 25%v/v under the following non-EGR conditions: (1) Constant fuelling rate, which resulted in progressively increasing in-cylinder average air/fuel equivalence ratio (λ) with increasing charge oxygen content and (2) Increased fuelling rate to keep constant in-cylinder average air/fuel equivalence ratio. The theoretical results of this investigation showed a significant reduction of exhaust soot and a small improvement of brake specific fuel consumption (BSFC) compared to base diesel operation. However, at all cases of oxygen-enriched diesel operation, a considerable deterioration of NO emissions was observed emerging the need for the application of a NO reduction technique. Hence, a second computational study was conducted for the aforementioned oxygen mole concentrations considering variation of high-pressure cooled EGR rate from 0% to 30%v/v under two different engine operating modes: (1) Constant inlet pressure, which resulted in progressively decreasing in-cylinder average air/fuel equivalence ratio with increasing EGR rate and (2) Increased inlet pressure to keep constant in-cylinder average air/fuel equivalence ratio (λ). The theoretical results of the combined use of air oxygen-enhancement and exhaust gas recirculation showed lower soot and NO emissions for EGR rates higher than 20%v/v compared to conventional diesel operation, which were accompanied by limited penalties in specific fuel consumption. These effects were more characteristics in the case of increased inlet pressure (i.e. constant air/fuel equivalence ratio). Hence, it appears that the oxygen-enrichment of the intake air stream and the utilization of high EGR rates provide a promising solution for reducing soot and NO emissions with imperceptible penalties in brake efficiency of commercial HD diesel engines.

ENGINE SIMULATION MODEL

The engine simulation tool, which is used in this study to perform the theoretical investigation of the effects of intake air oxygen-enrichment and EGR, has been successfully used in the past to describe the operational and environmental behavior of various types of HD diesel engines under operation with high-temperature or cooled EGR [28,29,30,31,32]. A comprehensive description of the multi-zone engine model used for conventional diesel operation [30] and for diesel operation with either high-temperature or cooled EGR [28,29,31,32] has already been provided by authors. Thus, only a brief outline of its main principles and components is presented in the following to facilitate understanding of the influence of air oxygen-enrichment and EGR on the prime mechanisms affecting combustion and pollutant formation. The simulation covers the entire engine cycle taking into account the gas exchange process.

Brief Description of Zone Formation

The development of the engine simulation code is based on a 3-D multi-zone combustion model capable of predicting the in-cylinder combustion characteristics and pollutant formation [28,29,30,31,32]. The simulation covers the entire engine cycle taking into account the gas exchange period using the filling and emptying technique. Hence, the simulation model considers the following engine subsystems: (a) Engine cylinder, (b) Fuel injection system and (c) Gas exchange system.

According to the model, the fuel jet is divided after injection into discrete volumes called “zones”, in the three dimensions [28,29,30]. The number of zones in the axial direction depends on the injection duration and the adopted calculation time step. In the present study, a time step of 0.5°CA is employed whereas the fuel jet is divided into five zones in the radial direction and into eight zones in the circumferential direction. A representative description of the fuel jet distribution is given in [Figure 1](#).

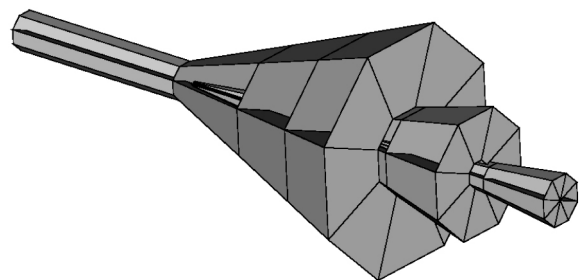


Figure 1. Fuel jet distribution into zones [30]

The first law of thermodynamics and the conservation equations for mass and momentum are used for the calculation of temperature and composition inside each zone. The pressure inside the engine cylinder is considered to be uniform. Most of the subsystems included in the model have been presented in detail by the authors in previous papers [28,29,30,31,32]. Hence, only an outline of each sub-model will be given below.

Heat Transfer

For the estimation of the characteristic velocity, necessary for the heat transfer calculations, a turbulent kinetic energy viscous dissipation rate $k \sim \epsilon_t$ model is used [4,33]. The heat transfer coefficient is estimated from a widely tested correlation in diesel engines as described in [34,35]. The heat exchange rate obtained is then distributed to the jet zones according to their mass, temperature and specific heat capacity [28,29,30].

Air Swirl

A hybrid scheme consisting of a solid body core surrounded by a potential flow region is considered to describe the motion of air as it enters the engine cylinder from the intake valve [36]. Then air swirl is estimated from the conservation equation of angular momentum.

Spray Model

After initiation of fuel injection, zones start to form and penetrate inside the combustion chamber. The zone velocity along the jet axis is obtained from correlations providing the penetration length of the fuel jet inside the cylinder [28,29,30,31,32]. The zone velocity at the jet periphery is estimated from the methodology described by detail in [28,37] using the radial distance of the zones from the jet axis. The effect of air swirl upon the jet is also considered, using the local components of air velocity in the radial and axial directions and momentum conservation equation in both axes.

Air Entrainment

Momentum conservation is adopted to estimate the amount of air entrained into the zones. The effect of injection pressure variation on the jet formation mechanism is taken into account by considering the independent initial velocity of each zone, based on the instantaneous injection and cylinder gas pressures.

Droplet Evaporation and Breakup

The injected fuel [38] is distributed to the zones according to the instantaneous injection rate. Inside each zone a chi-squared distribution is used to describe the distribution of the fuel droplet diameter. The evaporation process of diesel fuel is modeled using the theoretical approach suggested by Borman and Johnson [39].

Combustion Model

The amount of air entering a zone mixes with the evaporated fuel and the local reaction rate depends on the local concentration of fuel, oxygen and the local temperature. Ignition commences after an ignition delay period, which is estimated using the local conditions inside each zone [40].

Fuel Injection

In the present work, the injection pressure history was measured during experiment and used as an input to the simulation. From this, the instantaneous injection rate of fuel is calculated.

Gas Exchange

The method of “filling and emptying” is used to calculate the mass exchange rate between the inlet and exhaust manifolds and the engine cylinder [28,35,37].

Soot Formation and Oxidation

The semi-empirical model of Hiroyasu [41] is used to predict the soot formation rate in each zone [28,29,30,31,32]. The model is based on the assumption that the net mass of soot formed is the time integral of the difference between soot formation and soot oxidation rate. According to Hiroyasu's model [41], both rates of soot formation and soot oxidation depend on local temperature and mean cylinder pressure. In addition, the rate of soot yield depends on the local evaporated fuel mass whereas the soot oxidation rate depends on the local partial pressure of oxygen and local soot concentration.

Formation of Nitric Oxide

The formation of nitric oxide is controlled by chemical kinetics [35]. For its calculation, the extended Zeldovich's mechanism is used [28,29,30,31,32,35,37] in the present investigation.

ENGINE DESCRIPTION - TEST CASES EXAMINED

The theoretical investigation of the effect of intake air oxygenation and EGR was performed for a commercial turbocharged six-cylinder heavy-duty diesel engine. This is a direct injection diesel engine, which is equipped with a common-rail high-pressure fuel injection system. The examined heavy-duty diesel engine has a cylinder bore of 102mm, a piston stroke of 130mm and compression ratio 18.5:1 and its maximum power output is 170kW at 2200 rpm.

An experimental setup was installed at an engine development company and it comprised of the examined heavy-duty diesel engine, a high-pressure cooled exhaust gas recirculation system and measuring devices for recording various operational engine parameters and exhaust emissions. Hence, engine tests were performed at the 12 ESC operating points, which comprised of three engine speeds namely 1400,

Table 1. Values of engine speed, load and EGR rate for the 12 ESC operating points considered in the present analysis

Operating Point	Engine Speed (rpm)	Engine Load (%)	EGR Rate (%v/v)
A25	1400	25	10.06
A50		50	15.57
A75		75	13.36
A100		100	11.32
B25	1800	25	19.71
B50		50	17.49
B75		75	16.69
B100		100	16.37
C25	2200	25	19.28
C50		50	18.99
C75		75	19.10
C100		100	15.56

1800 and 2200 rpm and four engine loads at each speed namely 25%, 50%, 75% and 100%. At each operating point, a certain EGR rate was considered (see [Table 1](#) below) and measurements for the following engine parameters were obtained: Engine speed, in-cylinder pressure, brake power, fuel consumption, intake charge mass flow rate and tailpipe NO and soot emissions. The values of engine speed, load and EGR rate, which were considered at the 12 ESC operating points of the experimental investigation, are given in [Table 1](#).

Upon the initial experimental investigation at the aforementioned ESC operating conditions, additional measurements were obtained at B50, which corresponds almost to the middle of the operational range determined by the 12 ESC points. Measurements were received at B50 for engine performance parameters and exhaust emissions considering variation of EGR rate from 1% to 18%v/v.

The theoretical analysis performed in the present study comprised of two separate parametric investigations: The first one examined the effect of variable air oxygen content on HD diesel engine combustion characteristics and in-cylinder soot and NO formation. It also investigated the influence of intake air oxygen-enhancement on brake power output and specific fuel consumption as well as on exhaust soot and NO values. The second theoretical study examined the combined impact of intake air oxygenation and EGR on the brake power output, BSFC, soot and NO emissions of a HD diesel engine.

The theoretical examination of intake charge oxygen-enhancement was performed at 1800rpm and at 50% of full engine load (B50) without EGR for two different operating modes: (1) Constant fuelling rate, which resulted in increasing in-cylinder air/fuel equivalence ratio (λ) with increasing intake oxygen fraction and (2) Increased fuelling rate to keep constant in-cylinder average air/fuel equivalence ratio (λ). Initially, variation of intake air oxygen mole fraction from 21% to 25%v/v was considered at B50. At all oxygenation cases the fuel consumption and the inlet pressure remained the same with the corresponding ones of the conventional diesel operation at B50 (i.e. 18.25kg/h and 1.95bar). This examination was conducted to assess the influence of air oxygen-enrichment on HD diesel engine performance and emissions without changes in fuel injection rate and T/C system.

However, the increase of air stream oxygen resulted in the increase of in-cylinder air/fuel equivalence ratio changing explicitly the air/fuel stoichiometry inside engine cylinders. Hence, it was decided to eliminate the effect of varying in-cylinder mixture stoichiometry and investigate the influence of intake air oxygen-enrichment under constant equivalence ratio (λ) conditions. The in-cylinder average air/fuel equivalence ratio remained constant at all cases of intake air oxygenation by proper increase of fuelling rate whereas, the inlet pressure remained constant. The values of fuel consumption and in-cylinder average air/fuel equivalence ratio considered in the analysis of intake air oxygen-enrichment under constant and increased fuelling rate are presented in [Table 2](#).

As already mentioned above, the second theoretical study examined the combined effect of intake air oxygen-enrichment and variable EGR rate for assessing mainly the relative attenuation of NO emissions and the pertinent deterioration of exhaust soot and BSFC. This study also was divided in two different stages: First, engine simulations were performed using the multi-zone model for variable charge oxygen content from 21% to 25%v/v at B50. At each case of intake air oxygenation, variation of EGR rate from 0% to 30%v/v and constant inlet pressure were considered (i.e. constant inlet pressure mode). The progressive replacement of intake air stream by EGR at each case of oxygen-enrichment without varying the inlet pressure resulted in the reduction of air/fuel equivalence ratio (see [Table 3](#)) changing thus again, the stoichiometry of in-cylinder combustible mixture.

Hence, the second part of this theoretical investigation was devoted to the examination of intake air oxygenation and EGR under the same in-cylinder mixture conditions (i.e. constant λ mode) at 1800 rpm and 50% of full engine load (B50). This was made feasible by increasing the inlet pressure with increasing EGR rate at each case of air oxygenation in order to keep the in-cylinder average air/fuel equivalence ratio (λ) constant. The increase of inlet pressure in this case ranged from 1.95 to 2.9bar. Such pressure ratios are feasible by modern T/C systems, which are used in HD diesel engines.