FACULTY OF TECHNOLOGY

DEVELOPING TIER 5 ENGINE RAW EMISSIONS MODEL

Joni Kemppainen

Mechanical Engineering

Master's Thesis

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Tiivistelmä

Päästölainsäädännön uudistuminen on asettanut moottorivalmistajille entistä enemmän haasteita tiukentuvien päästörajojen myötä. Raja-arvojen alle pääsemiseen vaaditaan moottorilta modernia teknologiaa sekä monimutkaista pakokaasunpuhdistusjärjestelmää, mikä on lisännyt moottorin raakapäästöihin liittyvän informaation merkitystä. Etenkin moottorin tuottamien nokipäästöjen, sillä parhaan polttoainetehokkuuden saavuttamiseksi ja vikojen välttämiseksi partikkelisuodattimen regenerointi on suoritettava oikea-aikaisesti. Yleisin nokimäärän mittausmenetelmä kaupallisissa koneissa ja partikkelisuodattimissa on paine-ero suodattimen yli, minkä tarkkuus on tietyissä olosuhteissa riittämätön. Erilaisia malleja, joilla arvioidaan moottorin tuottamia raakapäästöjä, on kehitetty ohjaustarkoituksiin. Tämän työn tavoitteena oli kehittää raakapäästömalli tulevan Tier 5 päästölainsäädännön moottorille pakokaasunpuhdistusjärjestelmän ohjausta varten. AGCO:lla on ollut käytössä raakapäästömalli aiemminkin, mutta koska aiemmat päästörajat on saavutettu ilman pakokaasunkierrätysjärjestelmää (EGR), ei viimeisin päästömalli sisältänyt EGR:ää. Yksi työn haasteista, ja päätarkoituksista oli selvittää, kuinka EGR:n vaikutus päästöihin voidaan mallintaa. Lisäksi mallin kehittämisessä oli huomioitava, että sitä tullaan käyttämään raakapäästöjen arviointiin todellisissa ajo-olosuhteissa, minkä vuoksi sen laskennan täytyy olla nopeaa ja samanaikaisesti riittävän tarkkaa.

Työssä on perehdytty eri päästöjen muodostumisperiaatteisiin moottorin paloprosessissa, sekä tutkittu niihin vaikuttavien moottorinohjausparametrien merkitystä. Työn suoritusaikaan mainittu Tier 5 moottori on yhä ollut kehitysvaiheessa, joten malli on luotu hyväksikäyttäen olemassa olevaa testausdataa vanhemmasta moottorista. Malli on luotu Simulinkillä, mikä on MATLABin graafinen ympäristö, jolla voidaan mallintaa ja simuloida dynaamisia järjestelmiä eri teknisen laskennan osa-alueilla.

Luodulla mallilla on ajettu simulointeja tasaisissa toimintapisteissä, sekä off-road ajoneuvoille suunnitellulla testisyklillä (NRTC). Simulointituloksien perusteella, luotu malli on potentiaalinen vaihtoehto monimutkaisemmille fyysisiin ja kemiallisiin ilmiöihin perustuville malleille. Mallin tarkkuudessa on kuitenkin parannettavaa, sillä se luotiin kokonaan valmista mittausdataa käyttäen, eikä tarvittavia testejä mallin lopullista kalibrointia varten päästy suorittamaan. NO_x päästöjen osalta mallin tarkkuus oli tyydyttävä, sillä NRTC:n simuloinnissa arvioitujen NO_x päästöjen vastaavuussuhde mitattujen kanssa oli 0.9513. Nokipäästöjen kohdalla jäi huomattavasti enemmän parannettavaa, sillä korrelaatio mitattujen arvojen kanssa oli vain 0.7702. Heikko tarkkuus nokipäästöjen kohdalla johtuu noen voimakkaasti epälineaarisesta käyttäytymisestä transientti tilanteissa. Luodun mallin rakenne on hyvin yksinkertainen, sekä sen kalibrointi ei vaadi kohtuuttoman paljon vaivaa, minkä vuoksi se on potentiaaline vaihtoehto moottorin raakapäästöjen arviontiin reaaliaikaisissa sovelluksissa.

Asiasanat

Dieselmoottori, Päästöjen hallinta, Mallinnus, Moottorin raakapäästöt

ABSTRACT

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Abstract

The renewal of emission legislation has posed even more challenges to engine manufacturers with the tightening of emission limits. To get below the limit values, the engine requires modern technology and a complex exhaust aftertreatment (EAT) system, which has increased the importance of information related to the engine's raw emissions. Especially the soot emissions produced by the engine, because in order to achieve the best fuel efficiency and avoid faults, the regeneration of the particulate filter must be carried out in a timely manner. The most common method of measuring the amount of soot in commercial machines and particle filters is the pressure drop across the filter, the accuracy of which is insufficient under certain conditions. Various models to estimate the raw emissions produced by the engine have been developed for control purposes. The goal of this work was to develop a raw emission model for the engine of the future Tier 5 emission legislation for the control of the EAT system. AGCO has used a raw emission model before, but since the previous emission limits were achieved without an exhaust gas recirculation (EGR) system, the latest emission model did not include EGR. One of the challenges of the work, and one of the main purposes, was to find out how the EGR's effect on emissions can be modelled. In addition, when developing the model, it had to be considered that it will be used to estimate raw emissions in real driving conditions, which is why its calculation must be fast and at the same time sufficiently accurate.

The work has familiarized itself with the formation principles of different pollutants in the combustion process and investigated the importance of the engine control parameters affecting them. At the time the work was performed, the mentioned Tier 5 engine was still in the development phase and therefore the model was created using the existing test data from older engine. The model was created with Simulink, which is a MATLAB graphical environment that can be used to model and simulate dynamic systems in various areas of technical computing.

Simulations have been run with the created model at steady operating points, as well as with a test cycle (NRTC) designed for off-road vehicles. Based on the simulation results, the created model is a potential alternative to models based on more complex physical and chemical phenomena. However, the accuracy of the model can be improved, as it was created entirely using already existing measurement data, and the necessary tests for the final calibration of the model could not be performed. In case of NOx emissions, the accuracy of the model was good, as the correlation of the NOx emissions estimated in the NRTC simulation with the measured ones was 0.9513. In the case of soot emissions, there was much more room for improvement, as the correlation with the measured values was only 0.7702. The poor accuracy for soot emissions is due to the highly nonlinear behavior of soot in transient situations. The structure of the created model is very simple, and its calibration does not require an unreasonable amount of effort, which is why it is a potential alternative for evaluating raw engine emissions in real-time applications.

Keywords

Diesel engine, Emission control, Modelling, Control oriented model, Engine raw emissions

FOREWORD

This Master's thesis was conducted in cooperation with AGCO Power Oy in Tampere. The purpose was to develop model for estimation of raw engine-out emissions of Tier 5 diesel engine and to investigate how the effect of EGR on emissions could be modeled.

I want to thank the people in AGCO for offering their ideas and support on this topic during the work. Special thanks for Senior Dev.Eng. Tomi Virola and Dev.Eng. Maxime Toussaint for support and sharing their knowledge on this topic. Also, thanks to the Department Leader of Performance Development Ismo Hämäläinen for offering me this topic and the opportunity to work on this evolving field.

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Tampere, April 17th, 2023

Joni Kemppainen

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NOTATIONS & ABBREVIATIONS

ANN	Artificial Neural Network
CI	Compression Ignition
CO	Carbon monoxide
DPF	Diesel Particulate Fliter
EAT	Exhaust Gas Aftertreatment
ECU	Electronic Control Unit
EGR	Exhaust Gas Recirculation
NO_x	Nitrogen oxides
NRTC	Non-Road Transient Cycle
PM	Particulate Matter
λ	Relative air/fuel ratio

1 INTRODUCTION

Over the years, emission limits have been getting increasingly stringent, which has resulted in new challenges among engine manufacturers. Modern techniques such as common rail systems, EGR, chargers with variable turbine geometry (VTG), variable injection timing and many more have been adopted to diesel engines in order to achieve the emission limits together with low fuel consumption and high performance. This has led to an increase in the complexity of the hardware as well as the software and number of parameters needed to calibrate. (Riccio, Monzani & Landi, 2022.) Calibrating these complicated systems usually requires multiple experimental tests and therefore is time consuming and expensive. All this has led to an innovation in control systems and development of model-based controllers which can significantly reduce the cost and time of controller development and calibration. (Nikzadfar & Shamekhi, 2014.) The models that have been developed for control purposes can be referred to as control oriented or ECU-oriented models.

Although modern technologies allow optimizing the combustion for low emissions, exhaust aftertreatment (EAT) system is necessary to reach the stringent emission goals. The most common strategy to estimate the soot loading amount in real time applications in the DPF is to use pressure drop across the filter, which has some inaccuracies when the exhaust rate is low, or the passive regeneration takes place causing changes on pressure drop. To minimize the penalties in fuel consumption due to too frequent regenerations and prevent the DPF damage due to overloading, model-based approaches for the EAT system control have been established. (Huang, Hu, Guo & Zhu, 2019.) The subject of this thesis is to develop a raw emission model for the upcoming Tier 5 diesel engine to calculate the engine-out emissions in real time under transient operation. Raw emission model is basically simplified model of complex phenomena that lead to emission formation. The model will be used as input for the EAT system control unit and therefore the computational load must be kept low while maintaining sufficient accuracy. Since the Tier 5 emission legislation for off-road diesel engines will reduce PM and NO_x limits significantly, the soot and the NO_x models are the ones that require the most attention. Especially if the soot model is to be used for DPF regeneration control, predicting the engine-out soot load accurately under transient operation is important to avoid penalties in fuel economy and DPF system malfunctions. The engine-out emissions are affected by multiple operating factors, for example engine speed, injection quantity, injection timing, air-fuel ratio, EGR flow etc.

One of the main goals in this work is to come up with a way to model the effect of the EGR on transient emissions since the latest model used by AGCO did not include EGR. In addition, engine as a system contains several other variables, behavior of the emissions during transient operation is highly nonlinear and fundamentals of soot formation in combustion are still incompletely understood. All those things increase the challenge of the task.

For the modelling of transient emissions, it is important to understand the pollutant formation mechanisms and which engine parameters are affecting them. Therefore, kinetics of pollutant formation and phenomena during the combustion will be studied. In addition, different methods and possibilities for the emission modelling must be reviewed in order to find an appropriate approach for the application. Completing the model requires measurements for the engine through bench testing, but since the Tier 5 engine is still in development, in the model formulation, data from older engines will be utilized. It is possible to consider using simulated values for the final model if there is no time left for the Tier 5 engine bench testing.

2 POLLUTANT FORMATION

Diesel engine exhaust gas consists of four main pollutant emissions, which are carbon monoxide (CO), unburned hydrocarbons (HC), particulate matter (PM) which consist primarily of soot and soluble organic fraction, and oxides of nitrogen (NO_x), including nitric oxide (NO) and nitrogen dioxide (NO_2). The formation ratio of these pollutants is highly dependent on the engine technical solutions and operating parameters such as air-fuel ratio (AFR), injection timing, EGR rate, fuel distribution, temperature etc. (Resitoglu, Altinisik & Keskin, 2014.)

2.1 NO_x formation

The NO_x emissions from diesel combustion are formed when atmospheric nitrogen is oxidized by the oxygen contained in the intake air under high temperature. In the formation process, the nitric oxide (NO) is the dominant component generated in combustion. The oxidation reactions of nitrogen to form NO can be described by Reactions 1-3 according to the extended Zeldovich mechanism.

$$O + N_2 \leftrightarrow NO + N \tag{1}$$

$$N + O_2 \leftrightarrow NO + O \tag{2}$$

$$N + OH \leftrightarrow NO + H \tag{3}$$

In CI engines the concentration of NO_2 can be 10 to 30 percent of the total exhaust NO_x emissions. As the NO is formed in the flame zone in cylinder, it can be quickly converted to NO_2 through Reaction 4.

$$NO + HO_2 \rightarrow NO_2 + OH \tag{4}$$

Highest NO_2/NO ratios occur when the engine is operated at light load and cooler regions in cylinder, which can stop the conversion back to NO, are widespread. Otherwise, the NO_2 can be converted back to NO via Reaction 5.

$$NO_2 + O \rightarrow NO + O_2 \tag{5}$$

These kinetic formation mechanisms of NO and NO_2 are made assumptions regarding to equilibration, but the complexity of diesel engine combustion process has great impact on the NO_x formation. The initial NO formation rate can be expressed with temperature dependent Arrhenius equation (Equation 6). From the equation, it can be seen that the combustion temperature has exponential effect on NO_x formation rate.

$$\frac{d[NO]}{dt} = \frac{k_1}{T^{0.5}} e^{-k_2/T} [O_2]^{0.5} [N] \tag{6}$$

As the fuel is injected into the cylinder just before the combustion starts, the fuel distribution inside the cylinder is not uniform and the spontaneous ignition takes place in the area where the fuel-air mixture is close to stoichiometric, followed by flame propagation. Through the combustion process, mixing between already burned gases, air and lean and rich fuel vapor-air mixtures causes composition changes in gas elements that burned at specific equivalence ratio. The critical moment for NO formation is between the start of combustion and shortly after the peak cylinder pressure occurs, as the fuel mixture that is burned early in the combustion phase is compressed to a higher pressure and temperature, increasing the NO formation rate. (Heywood, 1988.)

When thinking about the formation of NO_x emissions in the combustion process, it is worth understanding how different engine input parameters affect the formation rate. Since most of the NO_x formation comes from atmospheric nitrogen, the oxygen concentration in the intake charge has a significant effect on NO_x formation. The NO_x formation can be controlled to some extent with dilution of the intake charge by EGR. The provided dilution by the EGR decreases the combustion efficiency and lowers the peak cylinder temperature resulting to lower NO_x emissions. However, reducing the NO_x emissions with EGR has limitations because excessive dilution results in poor combustion quality and thereby may increase CO, HC and PM emissions. (Heywood, 1988.) This trade-off between emissions, where changing a parameter in one direction has a positive effect for one and negative for another has been noticed to be strong especially between NO_x and soot.

NO_x emissions are also significantly affected by injection parameters. By delaying the injection timing, combustion process is retarded causing the combustion to occur later which leads to lower peak cylinder temperatures. Therefore, NO_x formation is reduced. (Heywood, 1988.) Another parameter, which is not directly used for NO_x control, is injection pressure. Since higher injection pressure has a positive influence on a spray formation and fuel atomization, it increases the combustion efficiency and thereby NOx formation. (Guzzella & Onder, 2010.)

2.2 Particulate matter emissions

Majority of diesel particulate emissions are a result of incomplete combustion of diesel fuel and lubricant oil. The particulates consist primarily of agglomerated carbon (soot) and soluble organic fraction, which is adsorbed by the carbon. In addition, some moisture and inorganic components such as sulfates can be condensed on the surface of particles. (Resitoglu et al., 2014.) The formation of soot occurs in combustion when the temperature in the cylinder is about 700-2500 °C. The pressures prevailing in the cylinder during soot formation are about 50 to 100 atm with sufficient air overall to fully burn all the fuel. The formation process is extremely quick and can be summarized in two phases, particle formation and particle growth. These phases happen in matter of milliseconds. (Heywood, 1988.)

The path to soot particle appearance is highly dependent on the formation temperature and in diesel combustion two mechanisms from aromatic and aliphatic HC compounds are manifested. First the precursors of soot are formed by oxidation and pyrolysis reactions of the fuel molecules. The most likely precursors include polycyclic aromatic hydrocarbons (PAH), acetylene and its higher analogues which then go through condensation or fragmentation reactions to create the first recognizable soot particles. The first created soot particles are very small, diameter of 2 nm or less and are often called nuclei. The fragmentation reactions take place in temperatures above about 1500 C where the aromatic rings and the aliphatic molecules break up into smaller hydrocarbon fragments and then form unsaturated molecules that eventually produce soot nuclei. The faster formation mechanism takes place at the lowest temperatures below about 1400 C where the pyrolysis of benzene creates macromolecules via gas-phase reaction. The pressure of these molecules grows until they condensate into micro droplets and eventually become nuclei. After the formation of the first soot particles the particle growth takes place via surface growth, coagulation and aggregation. (Heywood, 1988.)

It can be stated from the paragraph above that soot formation is an extremely complicated process. The high gas temperatures and pressures, turbulent mixing, complex fuel composition and unsteady nature of the process have made it difficult to understand the fundamental idea of soot formation in diesel engines and therefore, the soot formation process in diesel engine combustion remains incompletely understood. Therefore, it is useful to study the formation of soot with the cause and effect of different engine control parameters.

As NO_x emissions, also soot emissions are highly affected by the oxygen concentration in the intake charge. Reviewing the effect of EGR brings back the challenge of the trade-off between soot and NO_x as increasing the EGR rate above a certain threshold increases the danger of high soot emissions. The soot-NO_x trade-off is inherently connected to the Diesel cycle and has also been observed among other variables such as injection timing and injection pressure. While delaying the injection timing reduces NO_x formation it usually has the opposite effect on soot. By advancing the injection timing, combustion occurs earlier and hotter decreasing the soot formation. With early injection the oxidation of soot at later phase of combustion is also enhanced due to long period of the expansions stroke. High injection pressure results in good spray formation and combustion efficiency and is therefore beneficial for low soot emissions. (Guzzella & Onder, 2010.)

2.3 Carbon monoxide (CO)

Because diesel engines are often operated on a lean air-fuel mixture, they do not produce significant amounts of CO emissions. However, CO can be formed with certain conditions because it is product of an incomplete combustion. If there prevails an oxygen deficiency inside the cylinder, the fuel does not burn completely, and instead of generating nontoxic CO_2 from the carbon contained by the fuel, part of it forms into CO during combustion. These conditions can occur especially at the time of starting and sudden accelerations, where rich mixtures are required. Some CO can also be generated due to insufficient mixing of the fuel-air mixture. Insufficient mixing can be caused by weak swirl or turbulence in the combustion chamber or if the fuel evaporation is weak because the droplets are too large. (Resitoglu et al., 2014.) In addition, some CO is also formed throug soot oxidation reactions in the late phase of the combustion (Xi & Zhong, 2006).

Sarvi and Zevenhoven conducted research on the effects of different engine parameters on pollutant emissions of a large-scale diesel engine. The study revealed that CO emissions are significantly affected by the fuel type. In concern of the engine design and parameters, the injection nozzle design and injection timing were also noticed to have effect on the CO emissions. (Sarvi & Zevenhoven, 2009.)

2.4 Hydrocarbons (HC)

Like CO, hydrocarbons are also products of incomplete combustion, though the reasons that cause HC emissions are different to some extent. As mentioned earlier, the combustion process of CI engine is extremely complex and therefore, there are multiple processes that affect the diesel engine HC emissions. Especially the heterogeneous type of injection into the cylinder is one of the factors that increases hydrocarbon emissions. (Heywood, 1988.)

The two main formation mechanisms for hydrocarbon emissions are called undermixing and overmixing. The overmixing phase takes place early in the combustion process during ignition delay. The fuel injected into the cylinder, where turbulent conditions prevail, is distributed into zones where the fuel/air equivalence ratio varies and the mixture furthest downstream of the fuel spray core becomes leaner than the lean combustion limit, fuel/air equivalence ratio $\phi_L \sim 0.3$. This over lean mixture cannot auto ignite or support the propagating flame that is ignited in the slightly lean-of-stoichiometric region of the fuel spray. Unburnt lean mixture can then be oxidized only through slower thermal-oxidation reactions which will be incomplete and therefore some unburned fuel, fuel decomposition products and partially oxidized products escape the cylinder. The amount of unburned HC emissions from these overmixed regions is highly dependent on the amount of fuel injected during ignition delay, thus the HC emissions are highest in operation conditions where the ignition delay is long. (Heywood, 1988.)

HC emissions caused by undermixing are produced from the fuel injected into the cylinder during combustion process and it occurs due to two different methods of fuel entering the combustion chamber. Either excess fuel is injected into the cylinder at operating conditions where over fueling emerges, or the fuel leaves the injector nozzle at low velocity. At the low velocity fuel injection, the biggest source of HC emissions is the nozzle sac volume which is left filled with fuel at the end of the injection process. As the combustion and expansion continues the fuel left to the nozzle sac is vaporized by the heat produced in the combustion process. This fuel vapor and possibly some large fuel drops mix with air slowly and may escape the cylinder unburned. In addition, the nozzle hole size has an effect on the amount of fuel that is exhausted unburned. Even though diesel engines operate mainly on lean mixtures, in transient conditions such as acceleration, over fueling may occur, which creates locally over rich regions in the cylinder while the combustion proceeds. These over rich regions partially mix with air or lean already burned gases and burn completely in the cylinder, but some remain too rich to support the flame and exit the cylinder unburned. (Heywood, 1988.)

In addition to overmixing and undermixing, quenching may contribute to HC emissions significantly depending on the amount of fuel impingement on cylinder walls. Quenching is also noticed to have a larger effect in cold conditions e.g., in engine warm up phase. (Heywood, 1988.)

3 REVIEW OF EMISSION MODELING

Various methods have been used in order to model the emissions of CI engine. The models can be divided into three categories, phenomenological, empirical and semi-empirical models. Phenomenological models are used to calculate the in-cylinder emissions based on a detailed analysis of the progress of the chemical and thermodynamic properties of the cylinder charge during the combustion process. The calculation is done using 3D-CFD, quasi-dimensional or zero-dimensional thermodynamic models, which use the chemical and thermodynamic properties of the in-cylinder content as input quantities. (d'Ambrosio, Finesso, Fu, Mittica & Spessa, 2014.) In the case of NO_x models, the extended Zeldovich mechanism is often used to calculate the NO_x emissions. For soot emissions, Hiroyasu's model, which consists of two equations, one for soot formation and other for oxidation during combustion, is commonly used. The problem with phenomenological models is that they often require large amount of calculative power, which makes them unsuitable for real time applications (Tschanz, Amstutz, Onder & Guzzella, 2010). Attempts to decrease the calculative burden have been implemented by developing mean value models, where instead of crank angle resolved values of the conditions inside the cylinder, their representative average values are used. Phenomenological mean value soot model developed by Boulouchos and Kirchen used the method mentioned above.

In empirical and semi-empirical models, the physical and chemical formation principles of emissions are not considered or are considered only in very simplified way (Tschanz et al., 2010). Therefore, detailed knowledge of physical and chemical processes inside the combustion chamber is not needed and the requirements of computing power remain low, which makes them suitable for real time applications (d'Ambrosio et al., 2014). Though empirical models require quite a large number of parameters to predict the emissions with sufficient accuracy (Tschanz et al. 2010). The model structure of these models can be polynomial or determined by artificial neural network (ANN) like the model developed by Ozener, Yuksek & Ozkan, who used ANN approach in their work for predicting engine-out emissions and performance parameters such as torque, power and brake specific fuel consumption. Results for the output prediction were good but the model was not tested in transient operation which has great importance when developing model for real time applications. The problem with ANNs is that the networks can be trained to generalize well within the training data range but lack the ability to accurately extrapolate if the input values do not stay in the training value range (Mathworks). In transient operation nominal steady state values do not always apply and variations appear, which requires the training data to include abnormal operating points.

In semi-empirical model approaches the physical or chemical parameters that affect the emission formation such as the adiabatic flame temperature or the heat release rate are combined with relevant engine operating parameters that can be measured directly, like empirical models. Because of this, semi-empirical models tend to have better accuracy than empirical models, while maintaining quicker calculation than phenomenological models. (d'Ambrosio et al., 2014.) E.g., Lee et al. developed semi-empirical model for soot prediction. The model took into consideration the fuel injection characteristics using zero-dimensional spray model based on the lift off length and equivalence ratio at the lift off length. Also, combustion duration was considered which required 3D CFD simulations to confirm the combustion time.

When selecting the modeling approach, the calculation time must be considered, meanwhile the emission prediction must achieve sufficient accuracy. It must be noted that increasing the model complexity increases the computational complexity. Common approach to model non-linear behavior in commercial engines is to use operating point dependent lookup tables and curves, which allows linking certain parameter calibration to a certain operating point or variations around it (Guardiola, Pla, Blanco-Rodriguez & Calendini, 2013). Guardiola et al. used the ECU oriented method for predicting NO_x emissions in real time. The created model used engine speed and fuel mass dependent lookup tables to reproduce the nominal NO_x emissions, where the effect of intake oxygen was presented by an exponential variation. Additionally, thermal loading, humidity and intake mass flow dependence of the emissions were modelled with tabulated factors. Similar types of exponential variation have been used to model transient soot emissions. E.g., Huang et al. modeled transient engine out soot emissions to estimate the DPF loading. The model based on the nominal steady state emissions, where the transient variation was acquired with exponential function depending on the difference of initial and steady state λ values. Schilling, Amstutz, Onder & Guzzella and Tschanz et al. presented promising methods to use lookup tables and effects of the relative variation of input variables on emissions to model the dynamic behavior of engine out emissions. The models are calculating the difference of the emissions to the set point relative base values using the relative differences of each input variable and the pollutant sensitivity related to that input.

When modelling the emissions of CI engine, one important issue is how to handle the strong nonlinearity of the emissions, especially PM emissions. In addition, the multiple input multiple output characteristics must be considered. The control-oriented models described in a paragraph above enable both of those requirements to be fulfilled with a fairly simple method, as the dependencies between the relevant inputs and emissions are easy to identify with bench testing. Another advantage of those kinds of approaches is that they can be used with the signals that are available in the engine ECU.

4 MODEL APPROACH

Different possibilities for modeling the engine-out emissions were assessed when choosing the modeling approach. Although models that are based on the physical phenomena and reactions in the combustion chamber can achieve very accurate prediction results, they often require cylinder pressure and temperature information which are not typically available in commercial engines. In addition, they require complex calculations which has a negative effect on the calculation speed. In some studies, artificial neural networks have performed well, but the model accuracy relies on the training data which leads to a problem of over-fitting and generalization. ANN's are also basically black boxes which makes it difficult to recognize how much each independent variable is influencing the dependent variables and the outcome of model. Because of the reasons stated above as well as the easy identifiability and simple programming, the operating point dependent modelling approach was selected for this model. The model proposed in this paper utilizes the principles presented in the works of Schilling et al., Guardiola et al. and Tschantz et al.

The model is developed with prioritizing the control purposes and the computational burden is kept low. Therefore, the model uses only signals that are available from the engine ECU in real time operation. In the development of the model, efforts have also been made to build the model so that its tuning does not require an unreasonable amount of time for bench testing and measurements. During the model development, existing measurement data collected from a turbocharged heavy-duty engine equipped with common rail direct injection and EGR has been used. All the data that has been used in the model identification and formulation has been recorded in AGCO Power's testing facilities.

4.1 Equipment and testing facility

The raw emission model is designed to estimate the emissions of a turbocharged (VGT) common rail diesel engine equipped with EGR, which is supposed to meet the limits of Tier 5 emission legislation. Because the development process of the engine in question is still in progress at the time of this work, the initial model has been created utilizing existing data of different engine. The test data used for model identification and formulation is selected from an engine that has certain similarities with the upcoming Tier

5 engine, which are e.g., common-rail direct injection, turbocharger and EGR system. Because of these criteria and the decent amount of collected test data, the model has been created by using data collected from an 8.4-liter turbocharged heavy-duty engine equipped with EGR. The way of thinking behind this choice was that due to certain similarities between the engines the created model can be used to estimate the emissions of the future Tier 5 engine once recalibrated. Technical information of the 8.4-liter engine is presented in Table 1.

Table 1 Test bench engine information

Manufacturer	AGCO Power
Model name	84 AWF
Technical data	8.4-liter inline 6
Injection	Common-Rail DI
Charger	Turbocharger
EGR	Cooled high pressure
Rated power	280 kW @ 2100 rpm
Rated torque	1650 Nm @ 1500 rpm
Emission class	Tier 4 final

The used data has been collected through bench testing, where the engine is coupled with dynamometer and equipped with various measuring devices and sensors for verification and calibration purposes. Description of the test bench setup is presented in Figure 1 and the most important measuring devices are listed in Table 2.

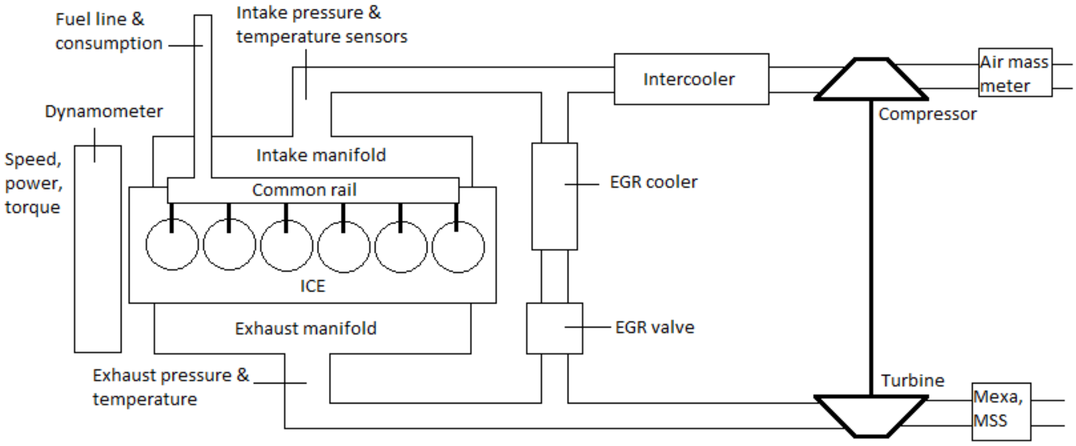

Figure 1 Schematic of test bench setup

Table 2 Measuring devices.

Sensyflow FMT700-P	Air mass flow meter
AVL 415S	Smoke meter
AVL Fuel Balance	Fuel consumption
AVL Indicom	Monitoring software
AVL 483 MSS	Micro soot sensor
Horiba MEXA	Exhaust gas analyzer
Horiba Stars	Automation system
INCA	Data acquisition
IMC	Bus transmitter
Kistler	Cylinder pressure sensor

The engine is coupled with eddy current brake and is controlled with Horiba Stars automation system, which allows the operator to run tests with the engine from simple manual testing to dynamic automated tests from single user interface. AVL 415S and AVL 483 are used for PM measuring. The AVL 415S is a smoke meter that uses filter paper blackening as its measurement principle and the range is 0 to 10 FSN. The AVL 483 is a micro soot sensor with a photoacoustic measurement principle and with a measuring range of 0.001 – 150 mg/m^3. The fuel consumption is measured with Fuel Balance which determines the consumption with high accuracy directly by measuring the time related weight decrease of the measuring vessel by means of a capacitive sensor. Horiba MEXA is a gas analyzer and can be used to measure multiple different pollutant emissions, such as NO_x, hydrocarbons, carbon monoxide and carbon dioxide from exhaust gases. It also includes a possibility to measure the EGR flow with the CO_2 measurements at the intake manifold and exhaust pipe. The operating parameters and multiple measurements that are collected with the wide range of sensors and analyzers are logged with Stars and INCA, which can be also used to change different calibration variables such as rail pressure from their reference values in the ECU and to postprocess, display and analyze the measurement data. Also, additional temperature and pressure sensors are used to record the ambient conditions.

The logging frequency can be changed in Stars between 10 seconds and 100 milliseconds. During transient tests, such as NRTC, high sampling rate is used to capture all the sudden variations in operating parameters and in emissions during transients. For steady state measurements such high sampling frequency is not needed as the measurements for each operating points are averages of the measured values in certain operating point and the transients between the operating points are neglected.

Therefore, sampling frequency of 1 second is enough in steady state measurements. INCA can be used to record different parameters available from ECU and the sampling rate can be under 1 ms depending on the measured variable.

The logged data from bench tests have been saved in excel sheets and is used in the model identification and formulation. The models have been created with Simulink, which is MATLAB's graphical environment that allows to model, analyze and simulate different dynamic systems using blocks and signal lines. The model can be simulated with MATLAB script, where the input variables are defined, and the results are plotted.

4.2 NOx model

In the operating point dependent model, the emissions in steady state operation can be estimated with measured values tabulated in lookup tables as a function of engine speed and fuel injection quantity. However, in transient operation, the emissions may differ significantly from the reference values measured in steady state conditions. These deviations in the emissions compared to the reference values can be explained with the deviations of different engine operating parameters from their base calibration values. Some of the control parameters that significantly affect the NO_x emissions are EGR rate, λ, and injection parameters such as injection timing and injection pressure. The mentioned parameters all affect the combustion efficiency and thereby the temperature inside the cylinder, which makes them potential variables for the NO_x model input signals and can be used in the estimation of transient NO_x emissions. Guardiola et al. showed a direct relationship between the intake oxygen concentration and fraction EGR/λ in their work on a control-oriented NO_x model. The EGR/λ, also referred as inert-gas rate, represents the portion of exhaust gas that has reacted with the injected fuel and does not contain oxygen available for combustion. It was also shown that there is an exponential correlation between the NO_x emissions and the fraction EGR/λ and it can be used as an exponential correction factor when modeling transient emissions. Similar correlation can be seen in Figure 2 where the normalized NO_x emissions measured in multiple different operating points are plotted as a function of EGR/λ.

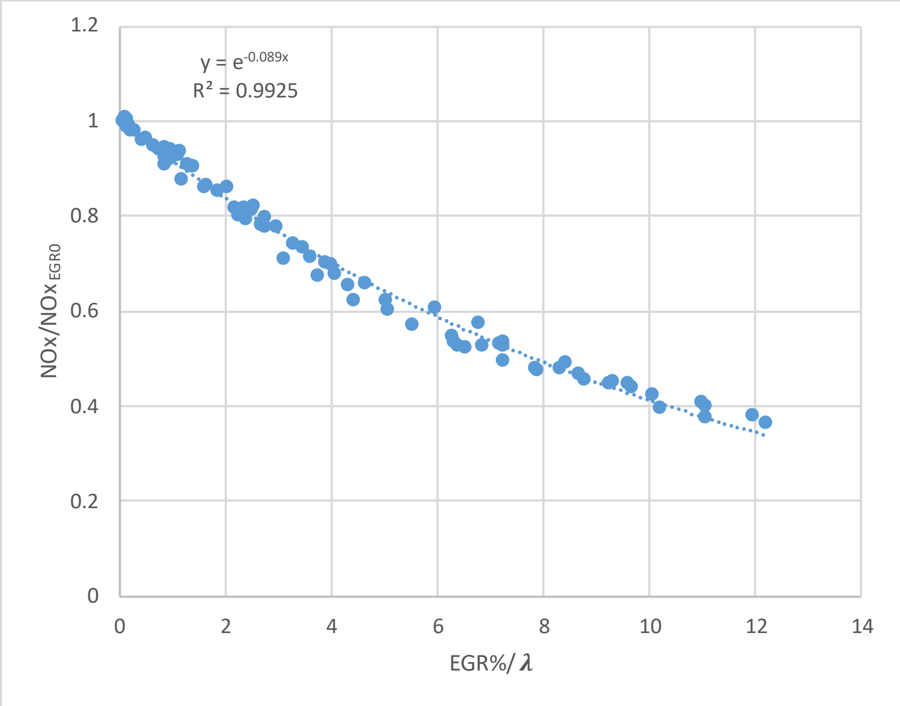

Figure 2 Normalized NO_x emissions as a function of EGR/λ for 98 different operating points.

With the same engine, EGR sweeps where the EGR rate has been varied from its reference value by adjusting the position of EGR valve, have been completed. The sweeps have been recorded at three different engine speeds, 1500, 1900 and 2100 rpm with 90% of the maximum load. Recorded NO_x emissions in relation to the reference value are tabulated as a function of EGR/λ and can be seen from Figures 3, 4 and 5.

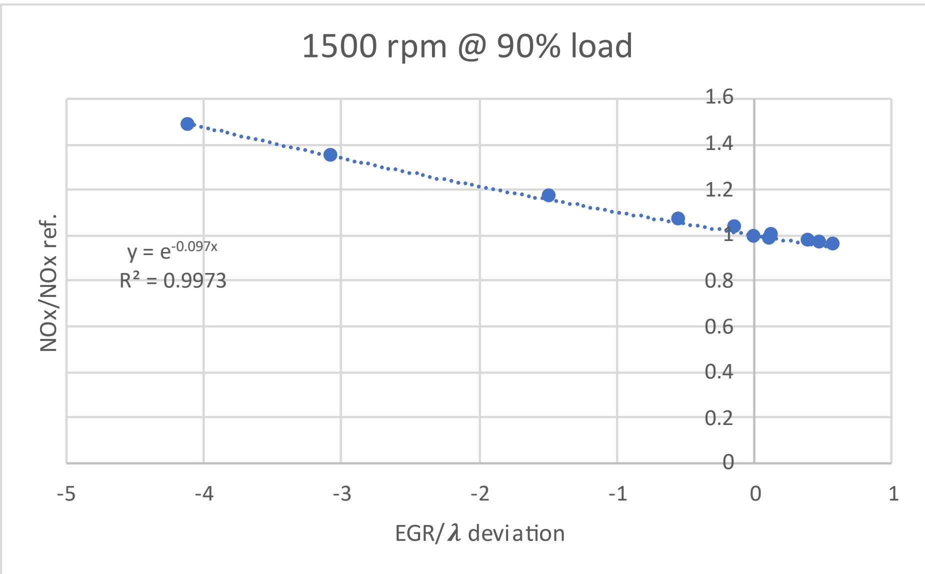

Figure 3 Effect of EGR/λ deviation on NO_x emissions at 1500 rpm and 90% load.

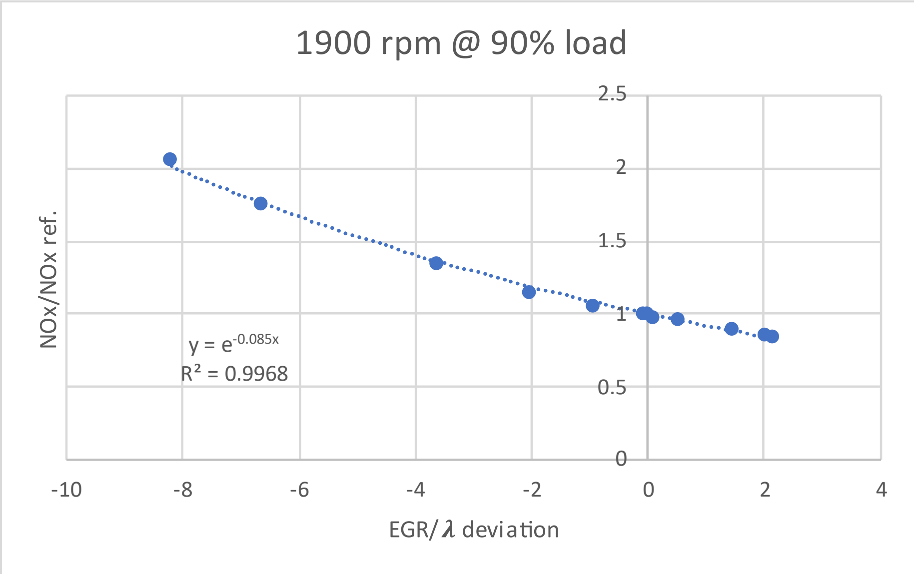

Figure 4 Effect of EGR/λ deviation on NO_x emissions at 1900 rpm and 90% load.

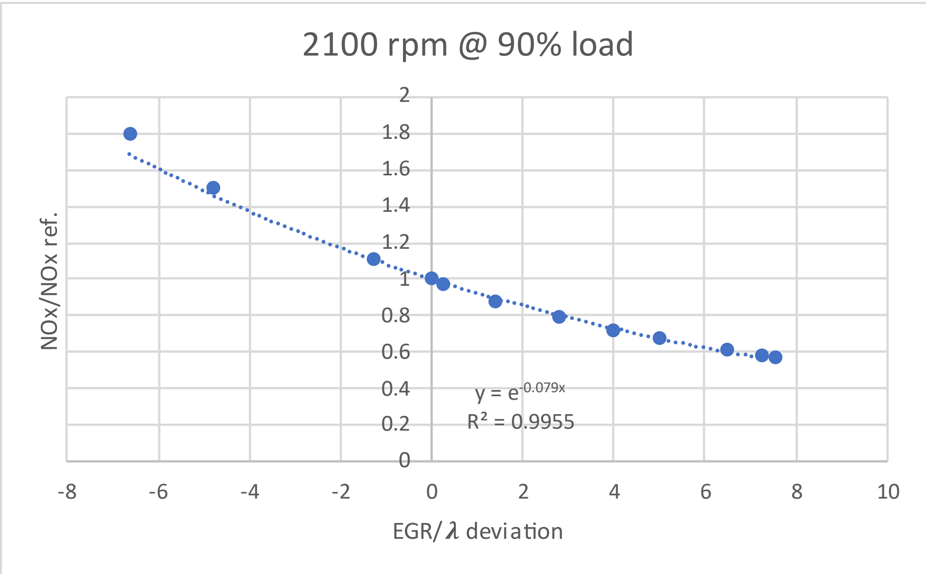

Figure 5 Effect of EGR/λ deviation on NO_x emissions at 2100 rpm and 90% load.

It can be stated based on the Figures 3-5 that the exponential relationship between the NO_x emissions and the inert-gas rate is strong in each measured operating point, but the steepness of the fitted curve varies between different operating points. Therefore, the exponential correction factor in the NO_x model requires operating point dependent calibratable coefficient.

Although the air-fuel ratio and the amount of introduced diluent have great influence on NO_x formation, injection parameters play a significant role as well. With delayed start of injection, the combustion is delayed and the peak temperatures inside the cylinder remain lower leading to lower NO_x concentrations. In turn, increasing the rail pressure enhances the vaporization of the fuel spray making the combustion process more efficient and increasing NO_x formation. In the method proposed by Schilling et al. the transient NO_x emissions are estimated with a set of input variables that are relevant in determination of NO_x emissions. The basic idea is to capture the deviations in the NO_x emissions related to the deviation of the selected input signal from its setpoint value, and then input signal deviations can be used to estimate the variations in the NO_x emissions during transient operation. In the work of Schilling et al. the relevant input signals were chosen with the help of sensitivity analysis, which showed that the injection parameters and air mass flow had a noticeable effect on the NO_x emissions. Tests where the rail pressure is varied have also been completed in AGCO Power's engine lab and the effect of rail pressure on NO_x emissions in various operating points is presented in Figure 6.

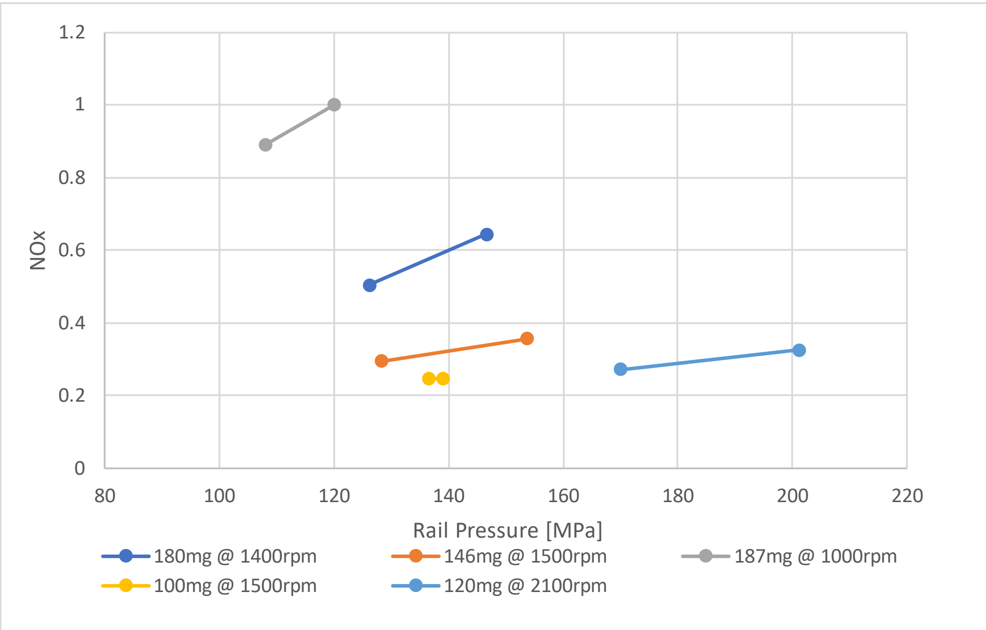

Figure 6 NO_x emissions as a function of rail pressure at various engine speeds and injection quantities (Normalized with the highest recorded value)

This model is an attempt to estimate the engine-out NO_x emissions using the methods described in the work of Guardiola et al. and Schilling et al. When considering the variables that have the most effect on transient NO_x emissions, the emissions can be described as a function of those variables according to Equation 7.

$$m_{tNOx} = f(n_{eng}, m_{finj}, m_{sNOx}, EGR, \lambda, p_{rail}, t_{inj}, \alpha_{SOI}), \tag{7}$$

where m_{tNOx} is the transient NO_x emissions estimated with the model, m_{sNOx} is the operating point dependent reference emissions, n_{eng} is the engine speed, m_{finj} is the fuel injection quantity, EGR is the EGR rate, λ is the relative air-fuel ratio, p_{rail}, t_{inj} and α_{SOI} are the rail pressure, main injection duration and main injection timing. The model is formulated so that the nominal NO_x emissions are multiplied with the exponential correction factor depending on the EGR/λ and corrections depending on the injection parameters. The NO_x model output is calculated using Equation 8.

$$m_{tNOx} = m_{sNOx} \times e^{k_{NOx} \times \left(\frac{EGR}{\lambda} - \frac{EGR_0}{\lambda_0}\right)} \times C, \tag{8}$$

where k_{NOx} is the operating point dependent coefficient and needs to be calibrated through bench testing. The subscript 0 after the variables refers to the reference values in steady state and those values are tabulated in lookup tables as a function of engine speed and injection quantity. C is the additional correction factor due to injection parameters and is defined in the following way.

$$C = C_{Prail} \times C_{SOI} \times C_{tinj}, \tag{9}$$

where C_{Prail}, C_{SOI} and C_{tinj} are individual correction factors for rail pressure, start of main injection and main injection duration respectively. Each individual correction factor can be defined as a sensitivity of the NO_x emission output value y with respect to the input variable value u. To calculate the sensitivities, normalized values of the deviations of input and output values are determined with Equations 10 and 11.

$$\delta u = \frac{\Delta u}{u_0} = \frac{u - u_0}{u_0} \tag{10}$$

$$\delta y = \frac{\Delta y}{y_0} = \frac{y - y_0}{y_0}, \tag{11}$$

where u and y are the input and output values, and variables with the subscript 0 are the reference values stored in lookup tables. Then, the sensitivities for each input variable can be calculated according to Equation 12.

$$\theta = \frac{\delta y}{\delta u} \quad (12)$$

Then the sensitivities can be stored to engine speed and injection quantity dependent lookup tables and the correction factor during transient operation caused by the deviation of input variables can be calculated with Equation 13.

$$C = \theta \times \delta u + 1 \quad (13)$$

Flow of the calculations and structure of the NO_x model is presented in Figure 7.

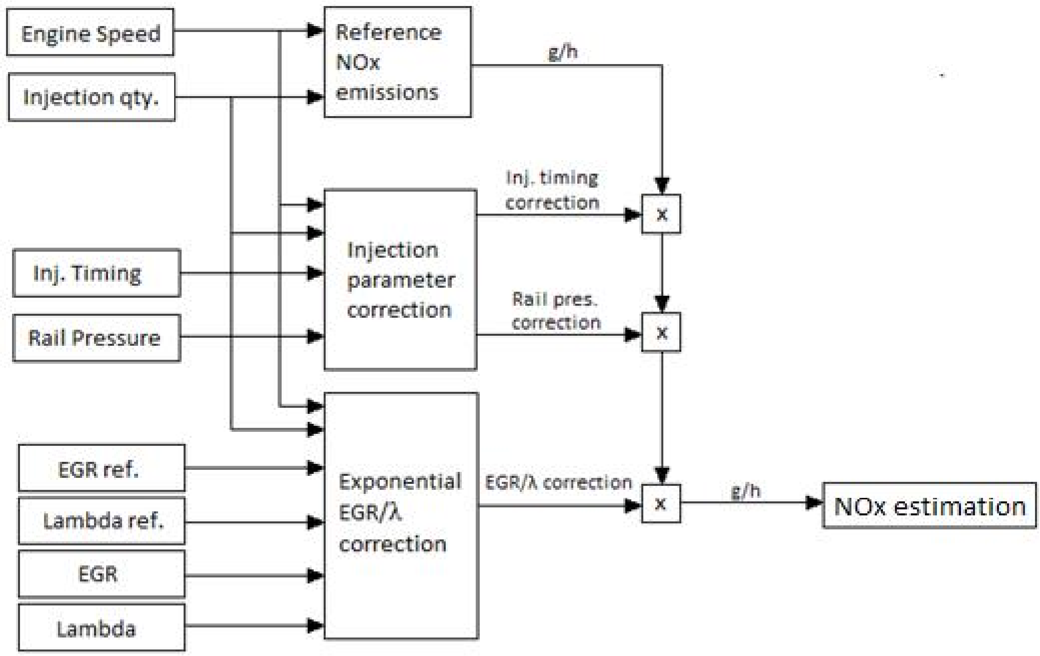

Figure 7 Structure of the NO_x model

The structure of the exponential correction factor will be presented later in Figure 15.

4.3 Soot model

Like NO_x emissions, transient soot emissions may also differ significantly from those measured in steady state operation. And since the soot emissions are product of incomplete combustion and highly affected by the combustion efficiency, many parameters that influence the NO_x emissions are also linked to soot emissions. In transient operation, frequent accelerations and decelerations cause variations in the operating parameters compared to the calibrated set point values. Because of these variations large momentary spikes can be detected in soot emissions during the transients. These spikes are typically caused by lack of oxygen inside the combustion chamber, which decreases the combustion efficiency and leads to incomplete combustion The lack of oxygen is typically caused by the lag of the air system while in turn the changes in fuel injection can be considered instantaneous. Therefore, in acceleration situations the relative air-fuel ratio drops momentarily which leads to soot spikes in the emissions. The size of these spikes varies significantly depending on both the acceleration and the current operating conditions. This was confirmed in the work of Huang et al. by adjusting EGR and throttle valve to create variations in air-fuel ratio at different operating points, which revealed that the decrease in the air-fuel ratio caused more sharp increase in soot emissions at conditions where the reference value of λ was relatively low compared to points where the reference λ was high.

Huang et al. used the deviation of λ from the reference value to create an exponential correction factor to model the transient soot emissions. However, the exponential correction did not consider the EGR rate, which has significant influence on the soot emissions due to lowered combustion efficiency. Galindo et al. presented that in addition to NO_x the inert gas rate has also strong relationship to soot emissions. This makes sense, since the λ is directly affected by the EGR flow when the introduced diluent decreases the oxygen content in the intake charge. The strong relation between soot emissions and EGR/λ can also be seen in data measured from the 8,4-liter engine in AGCO Power's engine lab and is presented in Figure 8.

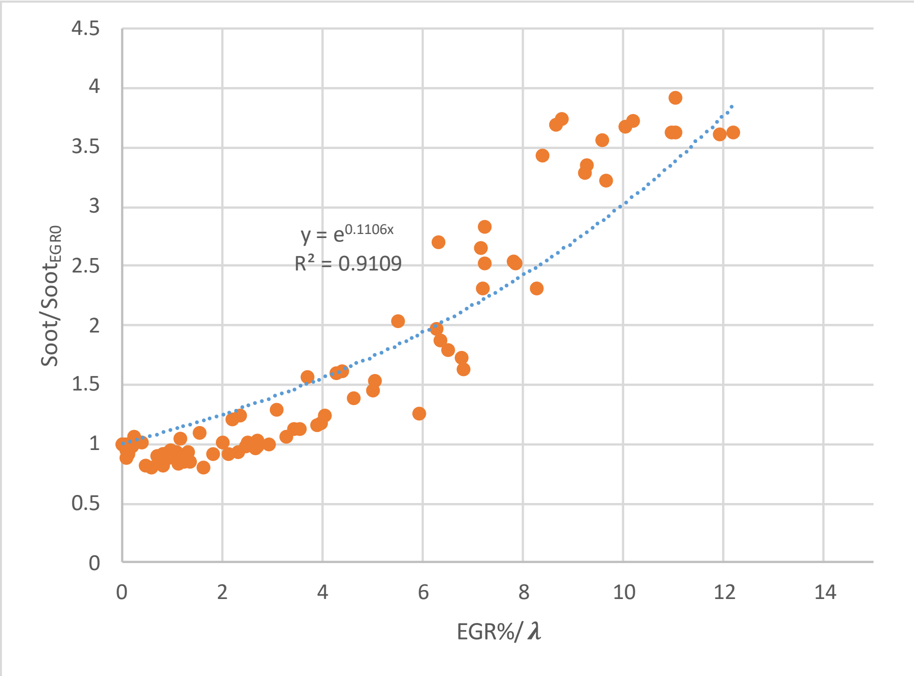

Figure 8 Soot emissions as a function of EGR/λ for 99 different operating points

When the soot emissions are fitted with an exponential curve a strong relation can be seen, but when compared to NO_x emissions, more dispersion is observed for soot. Also, the soot-NO_x trade-off is clearly seen as the soot emissions increase exponentially when the fraction EGR/λ grows while the NO_x emissions decrease. The soot-NO_x trade-off is presented in Figure 9.

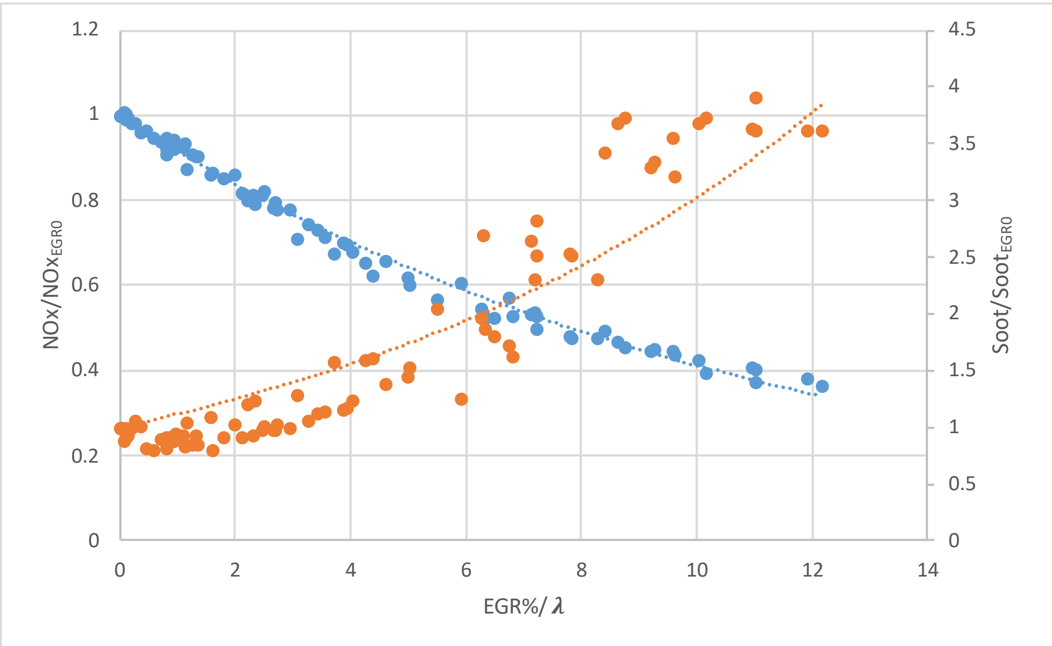

Figure 9 Soot-NO_x trade-off as a function of EGR/λ

Although there is more dispersion in the soot emissions, they can be presented as a function of EGR/λ using similar type of exponential correction as with NO_x. The soot emissions were also recorded in the EGR sweep tests on three different operating points with 90% of maximum load. Soot emissions normalized with the reference value on each operating point are shown in Figures 10, 11 and 12.

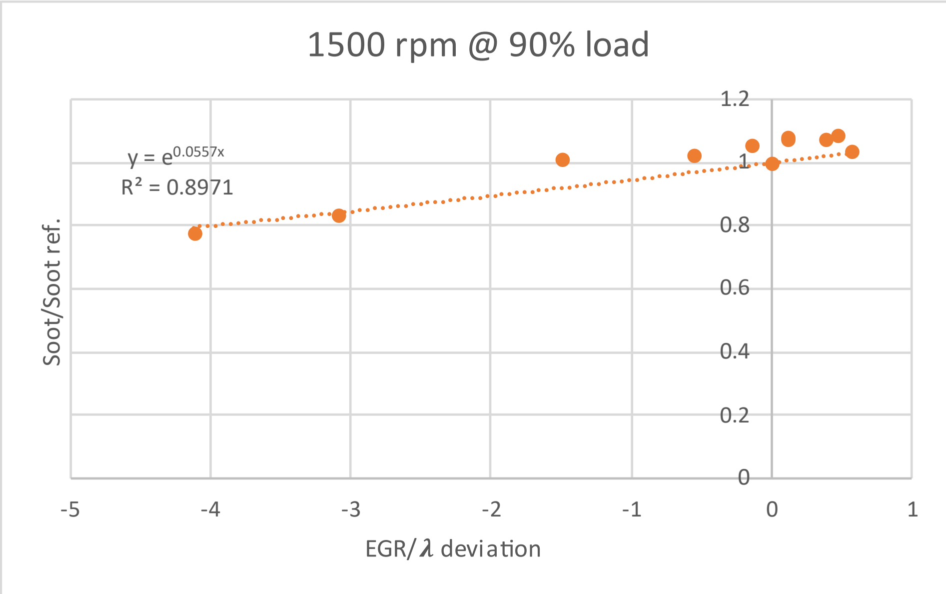

Figure 10 Effect of EGR/λ deviation on soot emissions at 1500 rpm and 90% load.

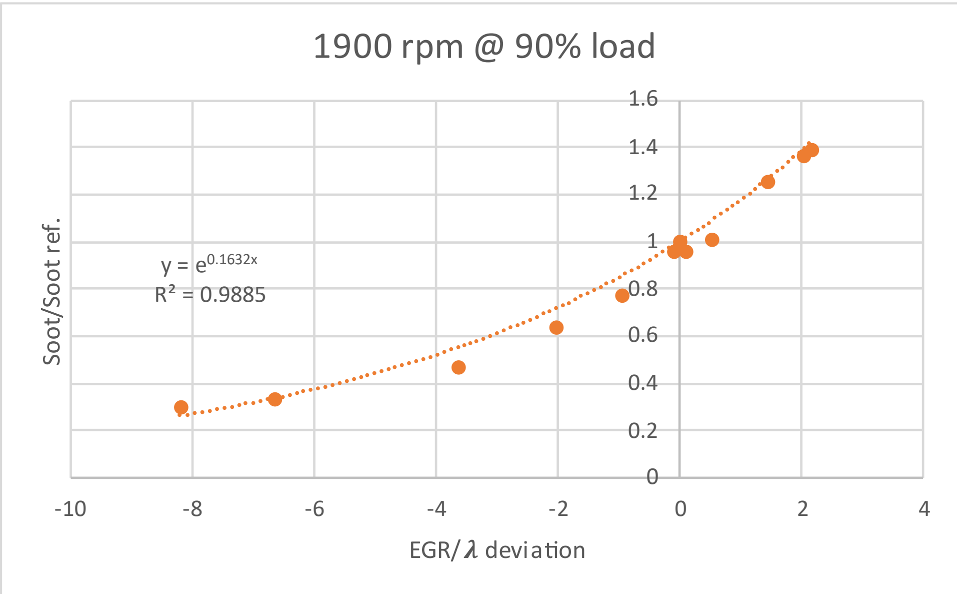

Figure 11 Effect of EGR/λ deviation on soot emissions at 1900 rpm and 90% load.

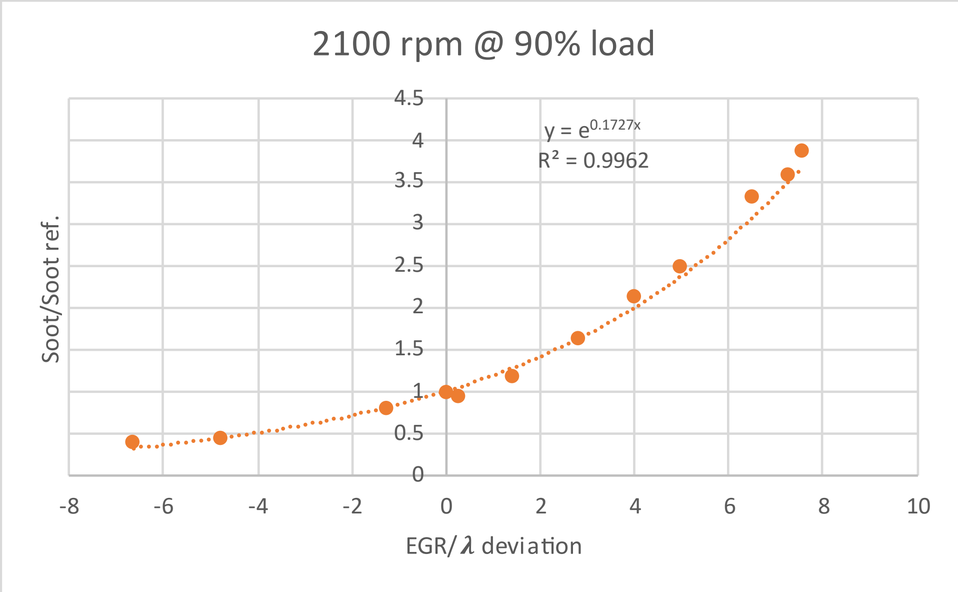

Figure 12 Effect of EGR/λ deviation on soot emissions at 2100 rpm and 90% load.

From figures 10-12 can be seen that the EGR/λ has strong exponential relation also with soot emissions and the steepness of the curve varies significantly in different operating points. Therefore, the model requires calibratable coefficient. Tschanz et al. used a similar method to Schilling et al. to estimate the transient soot emissions. In the model, injection parameters were used as input signals in addition to oxygen content and EGR rate, which is logical since the injection timing and pressure significantly affect the fuel spray characteristics and thereby the pollutant formation. Measurements where rail pressure is varied with different engine speeds and injection quantities show that increasing the rail pressure indeed reduces the soot emissions. Soot emissions as a function of rail pressure in different operating points are presented in Figure 13.

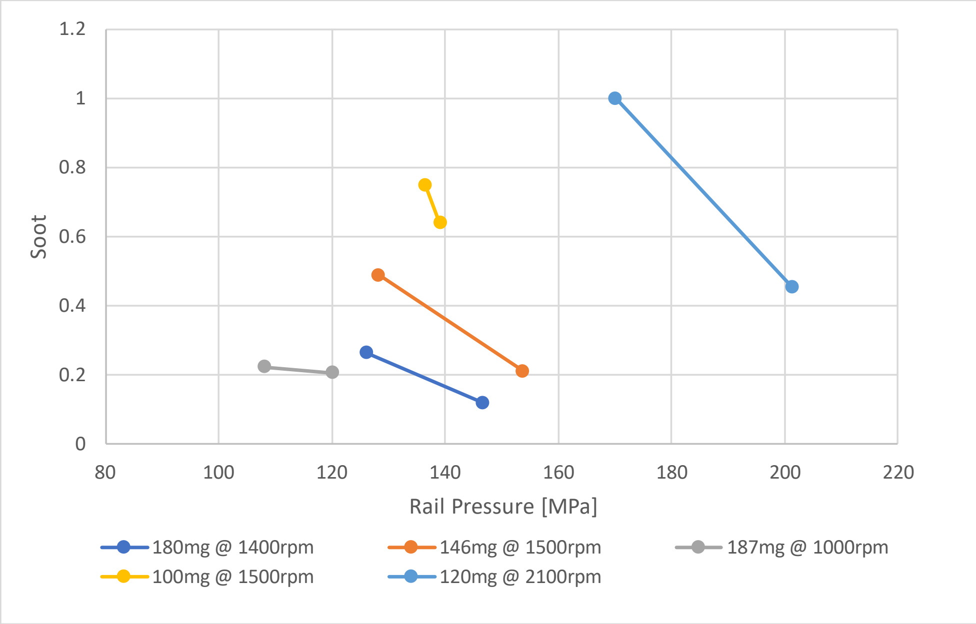

Figure 13 Soot emissions as a function of rail pressure at various engine speeds and injection quantities (Normalized with the highest recorded value)

In this paper, the soot model formulation is performed as a function of operating point dependent reference emissions and correction factors according to the following equation.

$$m_{ts} = f(n_{eng}, m_{finj}, m_{ss}, \lambda, EGR, p_{rail}, t_{inj}, \alpha_{SOI}), \tag{14}$$

where m_{ts} and m_{ss} stand for estimated transient soot emissions and steady state reference emissions respectively. Using the selected input variables, transient soot emissions are calculated by the model with Equation 15.

$$m_{ts} = m_{ss} \times e^{k_{soot} \times \left(\frac{EGR}{\lambda} - \frac{EGR_0}{\lambda_0}\right)} \times C, \tag{15}$$

where k_{soot} is the calibratable operating point dependent coefficient for the exponential correction factor and C is the additional correction due to injection parameters. The injection parameter corrections are calculated with same method as in the NOx model presented in Equations 10-13. The structure of the soot model is presented in Figure 14.

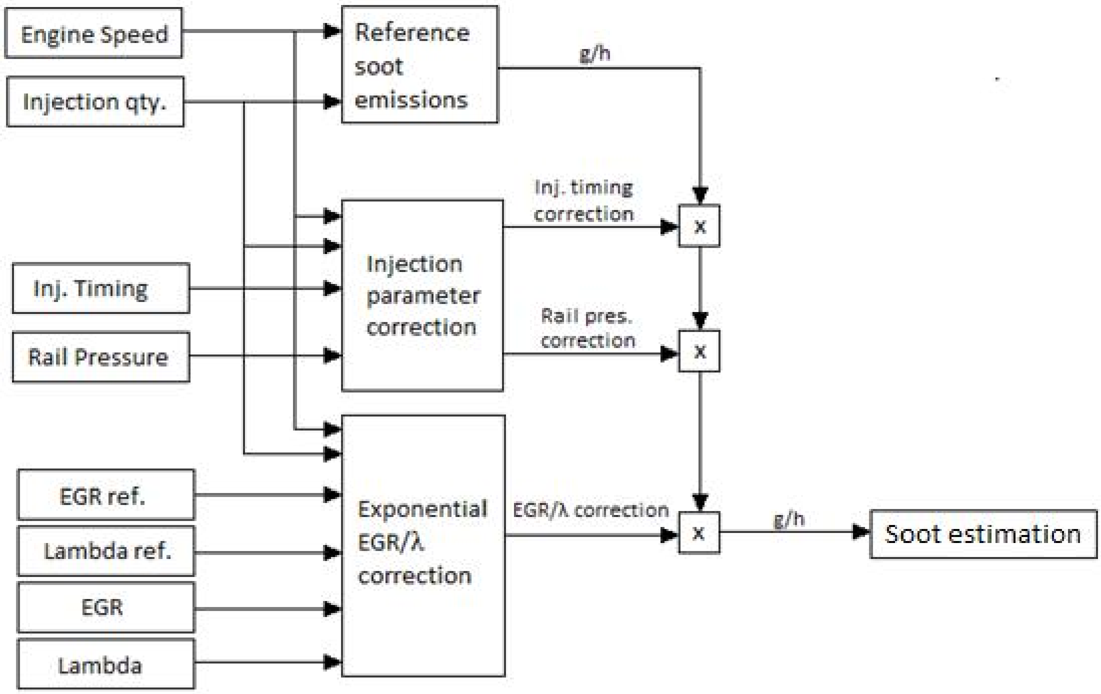

Figure 14 Structure of the soot model

In both NO_x and soot model, the exponential correction is implemented with similar way and the difference in the correction factor between the two models is caused by the coefficient k. Figure 15 presents the structure of the exponential correction factor.

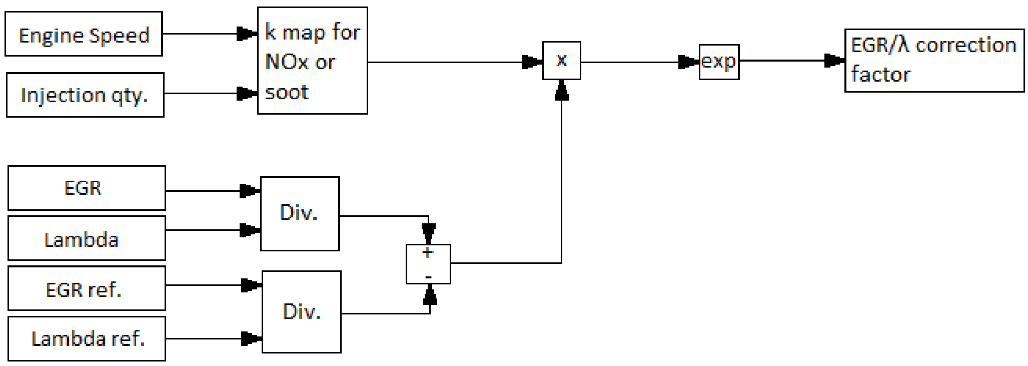

Figure 15 Structure of the exponential EGR/λ correction

4.4 EGR rate estimation

Estimation on engine-out NO_x and soot emissions has been implemented in a way that calculation can be done in real time using only signals available from the engine ECU. The engine-out emission model requires information of EGR rate, which is calculated as a ratio between EGR mass flow and intake mass flow according to Equation 16.

$$EGR = \frac{\dot{m}_{EGR}}{\dot{m}_{int}}, \tag{16}$$

where $\dot{m}_{EGR}$ is the recirculated exhaust gas mass flow and $\dot{m}_{int}$ is the total intake air mass flow and is measured by air mass meter. Since the EGR mass flow is not typically measured directly in commercial engines, an additional model for EGR flow estimation has been created. In addition, the fact that some of the data used in model formulation had EGR rate missing, and only the EGR valve position was recorded affected the decision to create additional model for EGR estimation. The EGR can be modeled as an orifice where the EGR valve is the area of the flow pipe which is varied by changing the valve position. The real area and the discharge coefficient, which varies with the valve area together, determine the effective orifice area. (Nyerges & Zöldy, 2020.) With these, the mass flow through orifice can be calculated using the well-known orifice equation (Equation 17) (Guzzella & Onder, 2010).

$$\dot{m}_{orifice} = A_{eff} \frac{p_{in}}{\sqrt{RT_{in}}} \psi\left(\frac{p_{in}}{p_{out}}\right), \tag{17}$$

where A_{eff} is the effective orifice area, R is the gas constant, p is pressure, T is temperature and the subscripts in and out stand for the conditions upstream and downstream of the orifice respectfully. The flow function $\psi(p_{in}/p_{out})$, can for many working fluids be approximated quite well with Equation 18. (Guzzella & Onder, 2010.)

$$\psi\left(\frac{p_{in}}{p_{out}}\right) = \begin{cases} \sqrt{\frac{2p_{out}}{p_{in}}\left[1 - \frac{p_{out}}{p_{in}}\right]} & for\ p_{out} \geq \frac{1}{2} p_{in} \\ \frac{1}{\sqrt{2}} & for\ p_{out} < \frac{1}{2} p_{in} \end{cases} \tag{18}$$

And by substituting the flow function in Equation 17 for orifice can be written as follows.

$$\dot{m}_{orifice} = \begin{cases} A_{eff} \frac{p_{in}}{\sqrt{RT_{in}}} \sqrt{\frac{2p_{out}}{p_{in}}\left[1 - \frac{p_{out}}{p_{in}}\right]} & for\ p_{out} \geq \frac{1}{2} p_{in} \\ A_{eff} \frac{p_{in}}{\sqrt{RT_{in}}} \frac{1}{\sqrt{2}} & for\ p_{out} < \frac{1}{2} p_{in} \end{cases} \tag{19}$$

The orifice equation is used to calculate the flow between two chambers with different pressures (Nyerges & Zöldy, 2020). For EGR system, where the flow takes place between the exhaust manifold and the intake manifold, equation can be written as is presented in Equation 20.

$$\dot{m}_{EGR} = \begin{cases} A_{eff} \frac{p_{exh}}{\sqrt{RT_{exh}}} \sqrt{\frac{2p_{int}}{p_{exh}} \left[1 - \frac{p_{int}}{p_{exh}}\right]} & for\ p_{int} \geq \frac{1}{2} p_{exh} \\ A_{eff} \frac{p_{exh}}{\sqrt{RT_{exh}}} \frac{1}{\sqrt{2}} & for\ p_{int} < \frac{1}{2} p_{exh} \end{cases}, \tag{20}$$

where p_{exh} is the pressure at exhaust manifold, p_{int} is the pressure at intake manifold, T_{exh} is the temperature at exhaust manifold and A_{eff} is the effective EGR valve area determined by the valve area and discharge coefficient (Equation 21).

$$A_{eff} = C_d \times A_{EGR}, \tag{21}$$

where the EGR area and the discharge coefficient varies depending on the EGR valve position. In addition, operating conditions such as pressure difference between exhaust and intake manifold and the flow turbulence affect the discharge coefficient. In theory, if all the variables except the effective EGR valve area are known, the effective area can be calculated with the help of orifice equation as follows.

$$A_{eff} = C_d \times A_{EGR} = \frac{\dot{m}_{EGR}}{\frac{p_{exh}}{\sqrt{RT_{exh}}} \sqrt{\frac{2p_{int}}{p_{exh}} \left[1 - \frac{p_{int}}{p_{exh}}\right]}} \tag{22}$$

For the data where EGR rate is measured, the calculated effective valve area is normalized with the maximum EGR valve area and can be plotted as a function of the EGR valve position. If the maximum EGR valve area is not known, its radius can be assumed to be some reasonable value such 0.01 m. and the maximum area is calculated with the valve radius r:

$$A_{max} = \pi r^2 \tag{23}$$

The normalized values of A_{eff} are plotted against the EGR valve position which reveals a strong nonlinear trend. The data can be fitted with a curve to model the valve opening characteristics and the effective area can be estimated as a product of the curve and maximum valve area. Then the A_{eff} can be replaced in equation 20 and the EGR flow can be calculated with Equation 24.

$$\dot{m}_{EGR} = A_{max} f(X_{EGR}) \frac{p_{exh}}{\sqrt{RT_{exh}}} \sqrt{\frac{2p_{int}}{p_{exh}} \left[1 - \frac{p_{int}}{p_{exh}}\right]}, \tag{24}$$

Where $f(X_{egr})$ is the EGR valve characteristics curve. The fitting of the curve is seen from Figure 16.

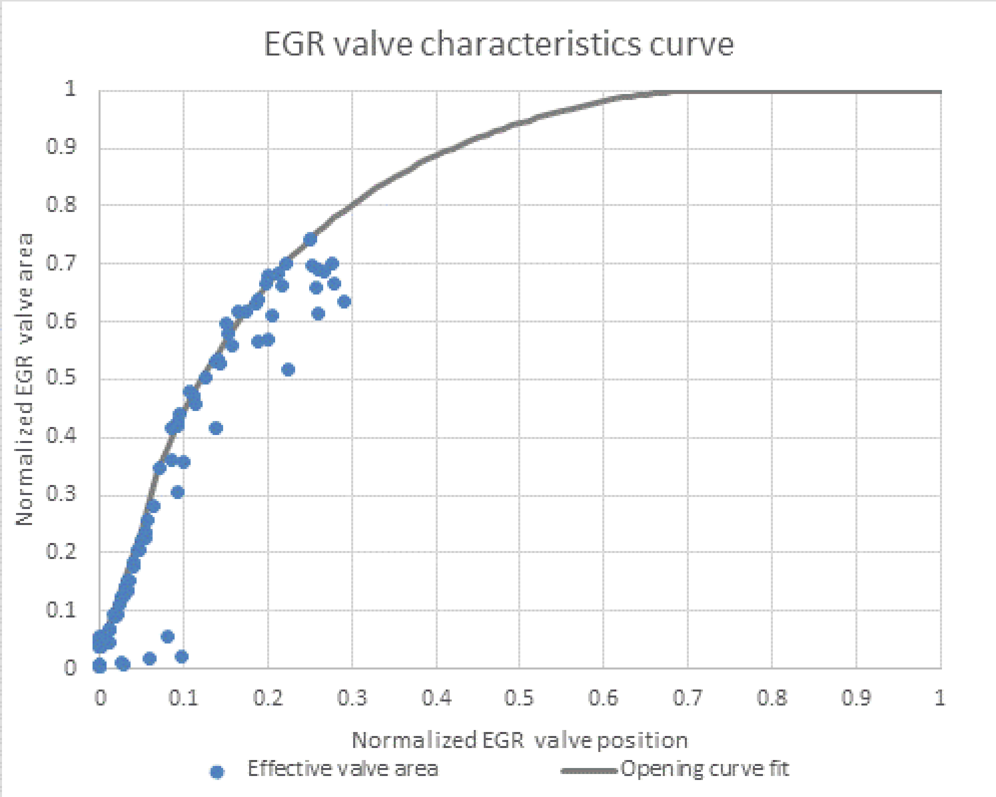

Figure 16 EGR valve opening characteristics curve.

Another method that could be considered for the EGR flow estimation is calculation as a difference of the engine intake air mass flow and fresh air mass flow:

$$\dot{m}_{EGR} = \dot{m}_{int} - \dot{m}_{air}, \tag{25}$$

where the intake air mass flow is calculated with Equation 26.

$$\dot{m}_{int} = \eta_{vol} \frac{p_{int}}{RT_{int}} \frac{V_d n_{eng}}{2}, \tag{26}$$

where η_{vol} is the volumetric efficiency of the engine, p_{int} and T_{int} are pressure and temperature at the intake manifold, V_d is volume of the engine and n_{eng} is the engine speed. By substituting $\dot{m}_{int}$ in the equation 25, EGR mass flow can be calculated with Equation 27. (Nyerges & Zöldy, 2020.)

$$\dot{m}_{EGR} = \eta_{vol} \frac{p_{int}}{RT_{int}} \frac{V_d n_{eng}}{2} - \dot{m}_{air} \tag{27}$$

4.5 Calibration

Since the basic idea of the model is using maps and curves to estimate the dynamic behavior of the emissions related to the set reference values, the model needs to be calibrated through bench testing. The reference values for input variables and emissions are gained by completing steady state measures for the whole engine operating area. Total of 244 stationary measurement points that have been completed with the 8.4-liter engine can be seen from Figure 17.

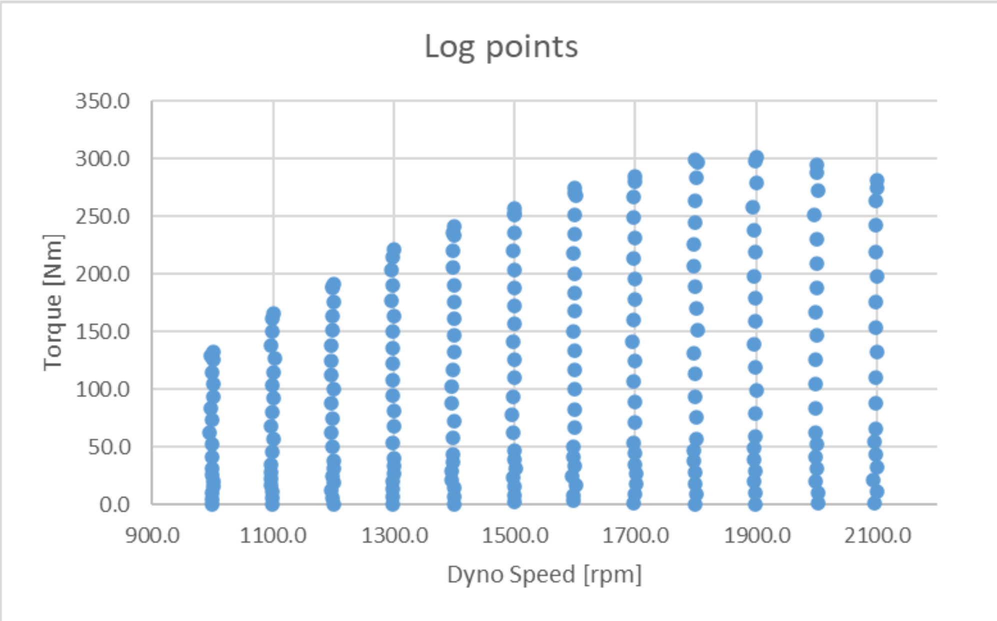

Figure 17 Operating points that have been used for reference values.

The emissions and input variables are then tabulated to lookup tables as a function of engine speed and injection quantity. When the engine is operating between log points, the reference values are obtained by interpolation between those points.

In the injection parameter corrections, the sensitivities Θ represent the ratios of the effect to the cause. In example in the NO_x model the sensitivity map Θ for the rail pressure is defined as ratio between the relative deviation of NO_x emissions from the reference value and the relative deviation of the rail pressure from its reference value. For example, if the reference value for rail pressure in certain operating point is 170 MPa and increasing the pressure to 180 MPa causes the NO_x emissions to increase from 1800 g/h to 1950 g/h, value for Θ is determined in following way by placing the values to the Equations 10-12.

$$\delta u = \frac{\Delta u}{u_0} = \frac{180MPa - 170MPa}{170MPa} = 0{,}059$$

$$\delta y = \frac{\Delta y}{y_0} = \frac{1950g/h - 1800g/h}{1800g/h} = 0{,}083$$

$$\theta = \frac{0{,}083}{0{,}059} = 1{,}41$$

Then the values for sensitivities are tabulated in lookup tables and the predicted outcome for the rail pressure correction is determined during the real time operation depending on the input deviation (Equation 13).

$$C_{prail} = \theta \times \delta u + 1 = 1{,}41 \times 0{,}059 + 1 = 1{,}083$$

And the model estimates the transient NO_x value by multiplying the reference NO_x emissions with the correction factor.

$$\dot{m}_{tNOx} = \dot{m}_{sNOx} \times C_{prail} = \frac{1800\ g}{h} \times 1{,}083 = 1949{,}4\ g/h$$

In ideal situation, the sensitivity values for the injection parameters are determined for each operating point. This though would require some time and it is possible that measurements at the extremes of the operating range and at some relevant operating points could be enough for sufficient accuracy. Then the missing values between the measured points would be gained by interpolation. Although the calibration procedure requires some time and effort, the similar structure of both soot and NO_x model enables the tuning of both models with same measurements.

The most critical part of the NO_x and soot model is the exponential EGR/λ correction since it is responsible for the largest variations during transient operation. In order to calibrate the exponential factor, tests in different operating points with variations in the EGR rate, in similar way that is done in Figures 3-5 and 10-12. Then the coefficients k_{NOx} and k_{Soot} can be determined by fitting an exponential curve for each tested operating point.

4.6 Simulations

Three created models, EGR, NO_x and soot were used to simulate steady state operating points and over the Non-Road Transient Cycle (NRTC). The EGR flow model was simulated with steady points to see the accuracy of the model, and if it is possible to be used with transient operation. EGR model correlation is shown in Figure 18.

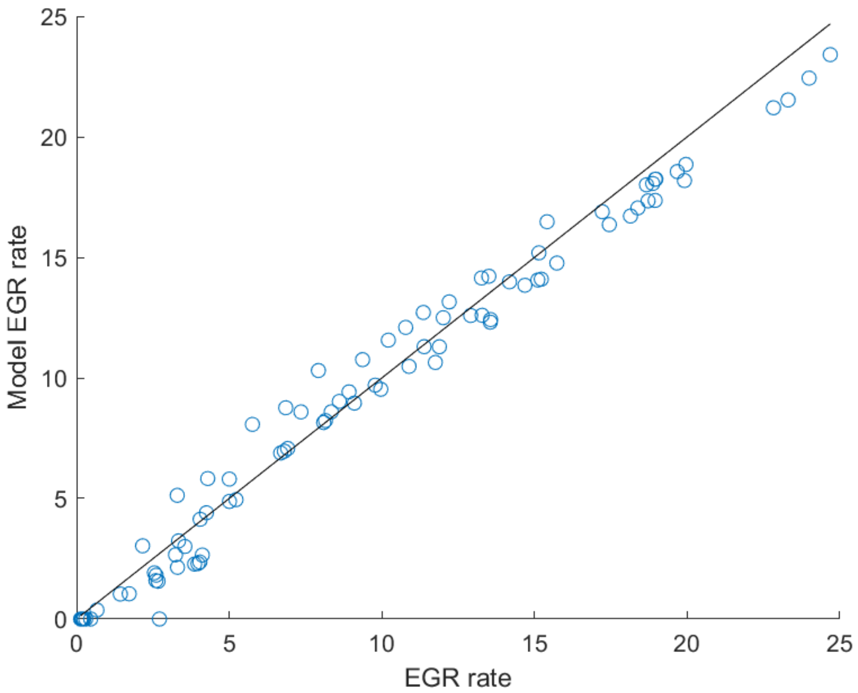

Figure 18 EGR model correlation with 98 different operating points.

Because data covering the whole engine operating area with recorded EGR rate was not available, the created EGR flow model was used to calculate the reference EGR rates for the full operating range in points presented in Figure 16. The EGR model was also used to estimate the EGR rate during the transient simulations. With calculated EGR rate values, full range of steady operating points were simulated with NO_x and soot models. Correlation of the NO_x emissions for steady state operating points is shown in Figure 19 and for the soot emissions in Figure 20.

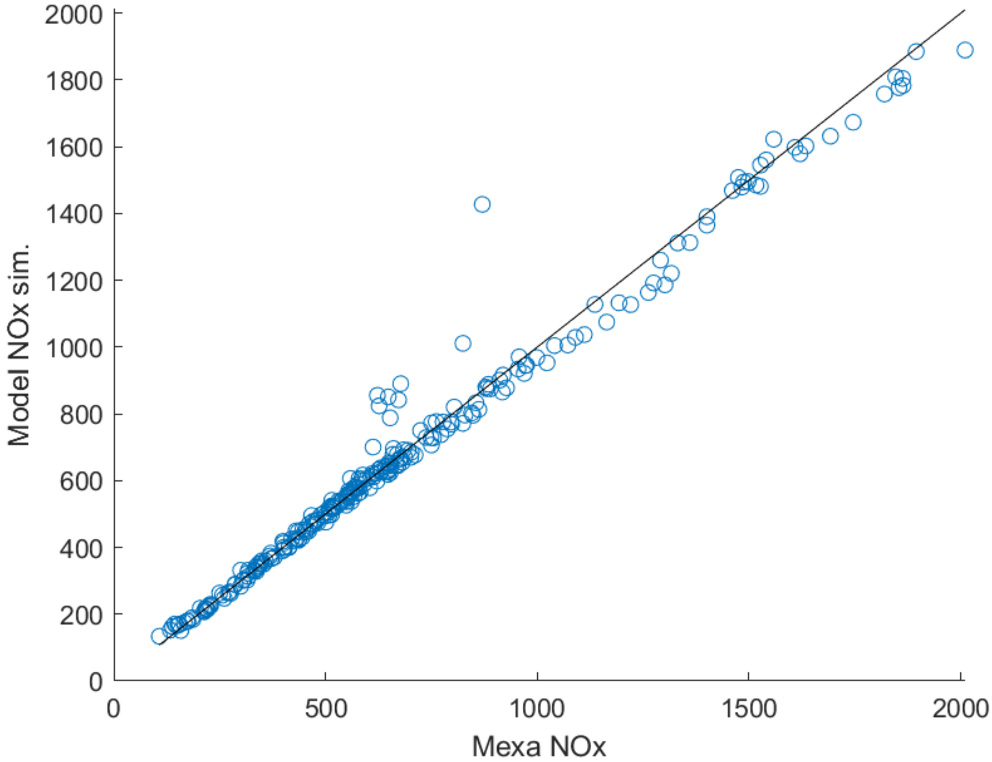

Figure 19 Correlation of NO_x emissions in 244 stationary operating points.

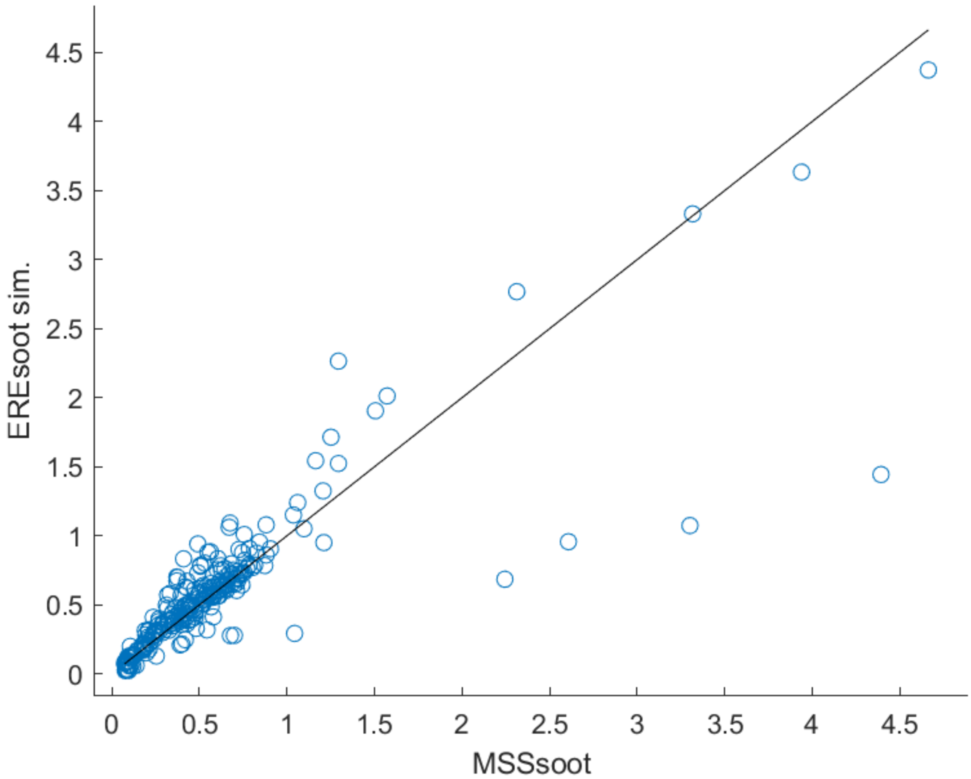

Figure 20 Correlation of soot emissions in 244 stationary operating points.

Simulations over the NRTC cycle were run and the results were plotted. Correlation during the cycle for NO_x model is presented in Figure 21 and the cumulative emissions and the trend of 5 second average are shown in Figures 22 and 23.

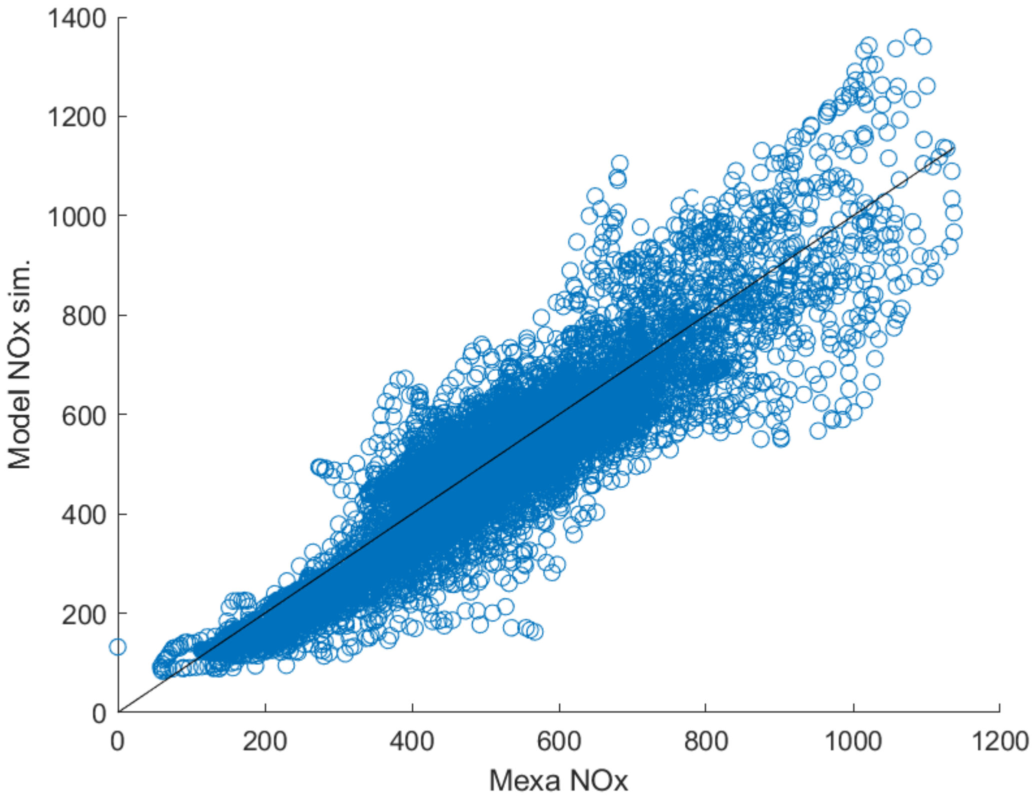

Figure 21 NO_x model correlation over the NRTC.

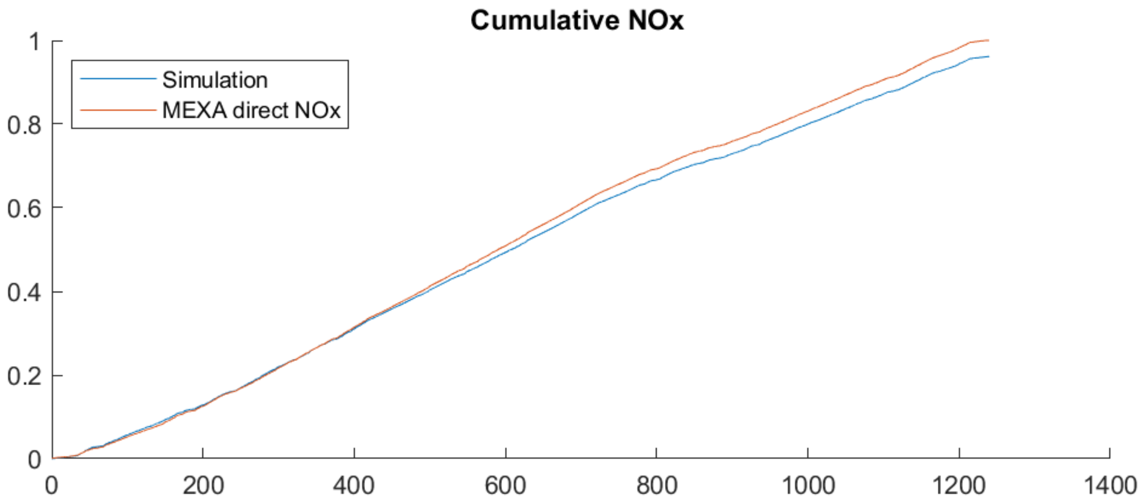

Figure 22 Normalized cumulative NO_x emissions over the NRTC.

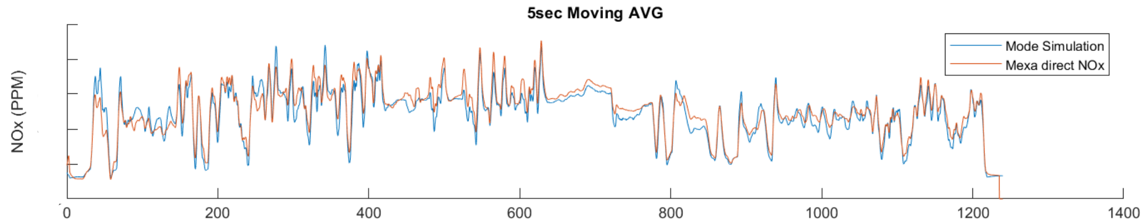

Figure 23 5 second average of the recorded and estimated NO_x emissions over the NRTC.

Results for the soot model simulation over the NRTC are presented in Figures 24, 25 and 26.

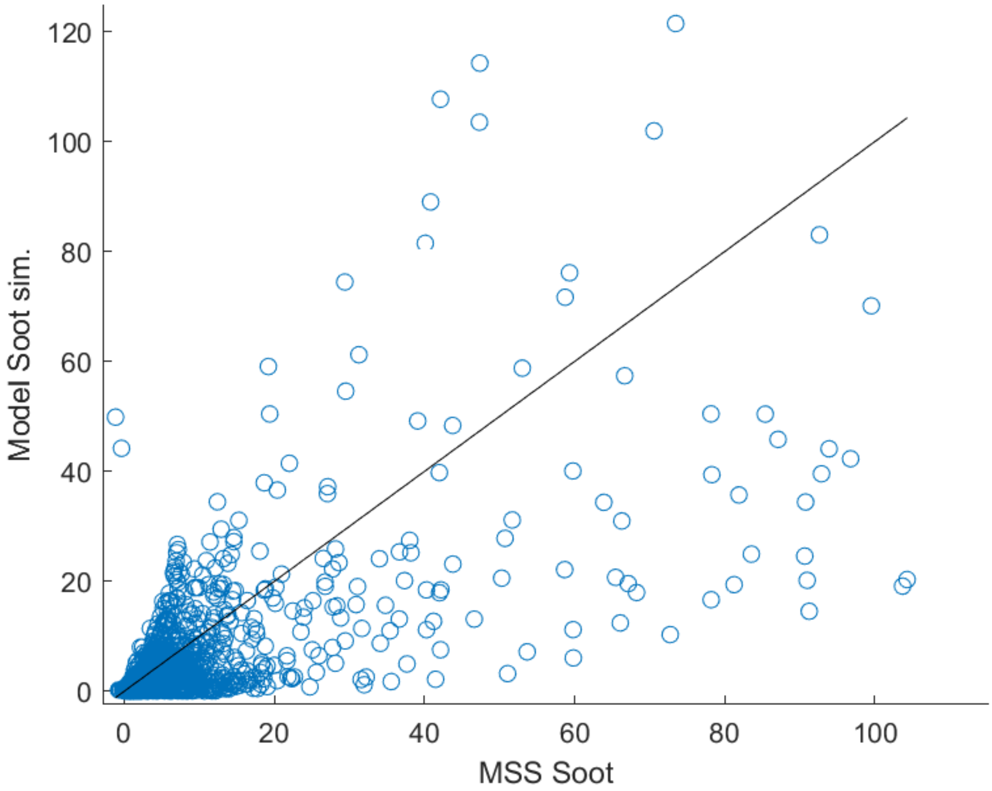

Figure 24 Soot model correlation over the NRTC.

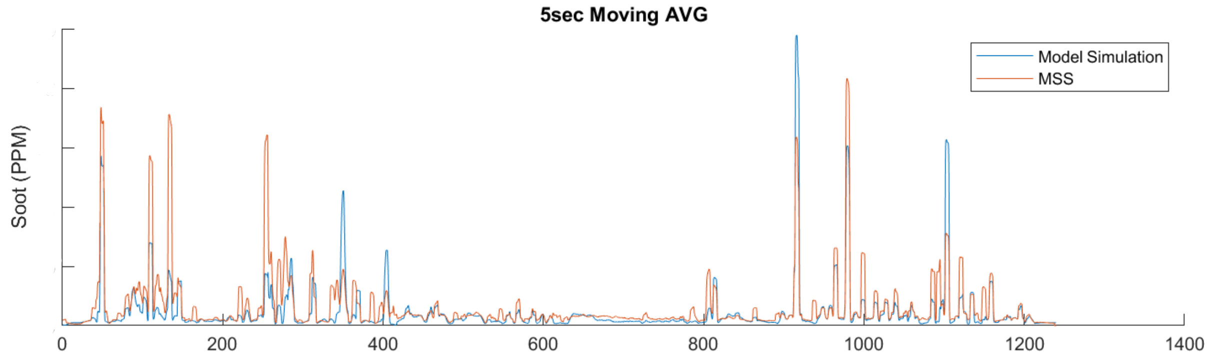

Figure 25 5 second averages of the recorded and estimated soot emissions over the NRTC.

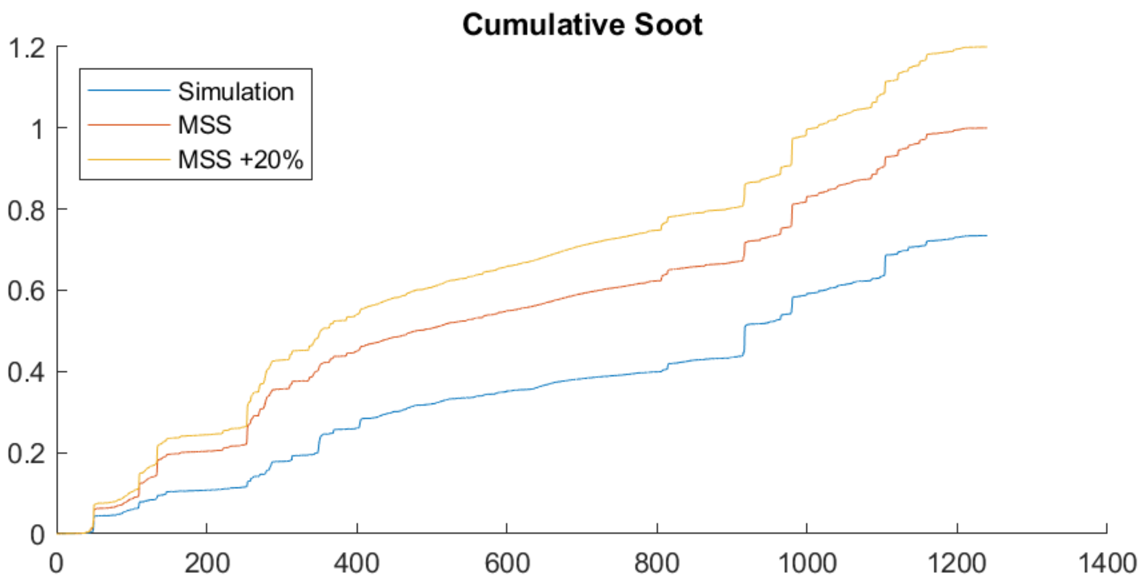

Figure 26 Normalized cumulative soot mass over the NRTC.

5 RESULTS

Three separate models, EGR flow, NO_x and soot have been created in aim of estimating the engine out pollutant emissions in transient operation. The EGR model was simulated over 98 different steady state operating points and the model accuracy can be seen from the correlation plot in Figure 18. The figure shows that in those operating points, the estimated EGR rate values set close to the regression line, but some deviation is noticeable. This is because the model is created on a basis of already existing data, and to achieve the best possible accuracy specific tests would be required. Most of the inaccuracy in the EGR model is caused by the discharge coefficient which varies depending on the valve position and the pressure difference between the exhaust and intake manifold. In addition, turbulence of the exhaust gas flow affects the gas discharge through the valve orifice.

The steady state simulations over the engine operating area for NO_x and soot emissions show good correlation with the recorded values. The accuracy of NO_x and soot models in stationary operating points is mainly depending on the calibration of the reference maps which were created with the test points presented in Figure 16. Since the simulation in those stationary points (Figures 19 and 20) shows good correlation with both NO_x and soot emissions, it can be stated that the calibration of the reference maps is on point. If there were clear differences between the recorded and tabulated values for the control parameters, it would show in the NO_x and soot model output. For example, if the tabulated lambda value in a certain operating point deviates from the recorded value significantly, it creates a visible difference in the emissions. But because the differences between the control parameters and their reference values are zero, or near zero, the values of the correction factors are one.

As expected, in transient simulation over the NRTC, the estimated values had noticeably more deviation to recorded values. However, with the NO_x model, fairly good accuracy was achieved given that the model was created entirely using existing measurement data. The correlation number of estimated NO_x emissions with the recorded values shown in figure 21 was 0.9513 and R^2 was 0.9050 which can be considered pretty good. The cumulative sum of NO_x in figure 22 shows that the model underestimates the actual emissions slightly over time and in the 5 second average plot the model underestimates and overestimates the emissions in some highs and lows. When compared to the earlier model that was used in AGCO, the NO_x prediction accuracy is close to same with the model developed here. With the older model, the correlation achieved with NO_x emissions was 0.9595, which is slightly higher than with this model. Though the model accuracy can be potentially increased with appropriate testing and tuning.

The soot model accuracy was expected to be lower than the NO_x model because of the highly nonlinear behavior of soot emissions during transients. The correlation plot (figure 24) reveals that the model accuracy is not as good as hoped and the emissions are either overestimated or underestimated. The correlation number over the NRTC for soot emissions was only 0.7702 and the R^2 was 0.5931. The over- and underestimation is clearly seen in Figure 25 where the 5 second averages of the estimated and recorded soot emissions are plotted. It shows that the errors in model estimation are happening during the soot spikes, the size of which is strongly depending on the operating conditions. Therefore, the soot spikes are difficult to predict with high accuracy, and some error is inevitable. When considering the purpose of the model, which is to use the estimate of the soot emissions as an input for the EAT system control, more important factor in the model accuracy is the capability to predict the trend over time. Cumulative soot emissions are presented in Figure 26, which shows that despite of the inaccuracies in the prediction results, the shape of the soot loading trend is quite similar between the estimated and measured soot emissions during the NRTC. When comparing the model accuracy to one developed by Tschanz et al., where the burned gas ratio and fresh gas mass were used as a coupled input with sensitivity map, the model developed in this paper has lower accuracy. They achieved a value of R^2 as high as 0.796 which means the correlation number of nearly 0.90. The difference in the model structure is mainly in the exponential correction factor used in this paper. The difference in accuracy can be partly explained by the fact that this model is developed with already existing test data, and actual calibration tests required by different coefficients and correction factors have not been completed. In AGCO, the older model which did not include the EGR rate and was used to estimate the raw emissions on engine without EGR, achieved a correlation of 0.8525 for soot emissions.

Although the estimation results of the models were not as good as hoped, they show the potential of the method used and that it can possibly be used as an alternate for more complicated prediction methods based on physical and chemical phenomena. Improving the accuracy of the models requires completing tests with which the effects of each variable at different operating points can be determined and verified. Another aspect which affects the usability of the created models is that they have been created using only data collected from warm engine. For example, the NO_x model output is needed when readings from NO_x sensors are not available, which is while the sensors are heating up. This means that the model is most often needed when the engine is still cold, and the emissions may be significantly different compared to hot conditions. The warmup phase affects all the pollutant emissions, because depending on the engine control, the injection patterns and timings may be different when the engine is cold. In addition, the cold cylinder walls and oil can affect the reactions inside the combustion chamber and the internal friction of the engine. Because of these factors, it would be wise to expand the model in the future so that the warmup phase is considered, for example as a function of engine coolant temperature or as different modes.

6 CONCLUSIONS

The subject of this work was to develop a real time capable model for predicting the raw emissions of the upcoming tier 5 off-road engine. The purpose is to use the raw emission model as an input for the EAT system to control the DPF regeneration and to replace the signal of the NO_x sensors in their absence. Because the future tier 5 emission legislation will reduce the NO_x and PM emission limits for diesel engines significantly, the soot and NO_x models were the ones requiring the most attention. One of the main problems in this subject was to find a method for estimating the effect of EGR flow to the pollutant emissions exiting the cylinder. In addition, the model's computational load had to be kept low for it to be suitable in real time applications.

As a result, various emission modeling methods have been studied in technical literature and publications, and raw emission models for NO_x and soot estimation have been developed. Created models have been developed by representing the transient emissions with the help of lookup tables and curves that need to be calibrated through bench testing. The nominal emissions of the created NO_x and soot models are presented with engine speed and injection quantity dependent lookup tables that are obtained from stationary measurements. The variations in emissions that occur during transient operation are attempted to capture with correction factors depending on the drift of input variables that are relevant in pollutant formation. The input variables used have been selected based on theoretical knowledge and observations presented in technical studies. The effect of the intake oxygen is modelled in both NO_x and soot model with an exponential variable by using the fraction EGR/λ, also known as inert-gas rate, which was shown to have strong relationship with both pollutants under consideration. Additional correction due to injection pressure and timing deviation was also included. The models have been formulated using already existing test data, and because from part of the used data measured EGR rate was missing, an additional model for the EGR flow estimation was created. The EGR model was based on the equation of flow through orifice between two chambers with different pressures because of its simplicity and that the required signals are probably available from the ECU. Another calculation method for estimating the EGR flow as a difference of intake air mass flow and fresh air mass flow was also presented, but it was not used in the simulations.

Simulations in stationary operating points and over the Non-Road Transient Cycle were completed and they revealed a good accuracy in case of the NO_x model, which had a correlation of 0.9513 with measured NO_x emissions over the NRTC. The correlation achieved was close to the number 0.9595, which was achieved with the old NO_x estimation model that did not include EGR. The soot model's accuracy has room for improvement since it achieved a correlation of only 0.7702 over the NRTC while the previous model had accuracy of 0.8525. Also, for the comparison, the model created by Tschanz et al., which has similarities with the model created in this paper, had R^2 value of 0.796 in transient simulations while the model at issue had 0.5931.

The emission model developing process was quite challenging as the goal was in developing the model for the future Tier 5 engine. And since the engine was still in development and required tuning and calibration, the necessary test data for the model was never obtained from the engine in question. Therefore, the model had to be formulated with the help of already existing test data from an older engine. The data used was selected from the engine which was assumed to have similarities with the upcoming Tier 5 engine. Some of those criteria were turbocharger and an EGR. In addition, with the fact that the model was created using old test data, some of the recorded tests had some input values missing, that are relevant for the models. One of the most relevant inputs in the case of the created models was EGR rate, which was missing from some data sets and only the EGR valve position was recorded, which is why the EGR flow model was created. In addition to the challenges mentioned, the fact that the author had no previous experience or knowledge about control-oriented models increased the difficulty of the work.

Although the model accuracies have room for improvement, it can be stated from the results that with appropriate tests for calibration, the described method can potentially be used for the real time estimation of NO_x and soot emissions. Also, must be noted that the developed models are simulated only with warm engine conditions, and since in the engine warmup phase cylinder walls are cold and the injection patterns and timing may be different from the normal operation, NO_x and soot emissions can be significantly different. Especially, because the NO_x estimation is required when the sensors do not work, which is basically when the sensors have not warmed up yet, an additional correction for cold engine must be considered. Another possible method to take account of different conditions could be multi-mode approach, when the model should be calibrated in different temperatures. In the future, the developed models can be easily updated and improved with changing or adding inputs that are used for the corrections as the user desires. Testing the accuracy of the models with the alternative EGR flow estimation method should also be considered. Developing models also for HC and CO emission estimation was originally in purpose, but with the encountered challenges there was no time for that, so it remains for further development in the future.

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