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Measuring and Predicting Transient Diesel Engine Emissions

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Academic thesis, which with the approval of Kungliga Tekniska Högskolan, will be presented for public review in fulfilment of the requirements for a Licentiate of Engineering in Machine Design. The public review is held at Kungliga Tekniska Högskolan, Brinellvägen 23 in room B3, 24th of March 2009 at 10:00.

Abstract

Due to its impact on human health and the nature surrounding us, diesel engine emissions have been significantly reduced over the last two decades. This reduction has been enforced by the legislating organs around the world that gradually have made the manufacturers transform their engines to today's complex high-tech products. One of the most challenging areas to meet the legislations is transient operation where the inertia in gas-exchange system makes transition from one load to another problematic.

Modern engines have great potential to minimize the problems associated with transient operation. However, their complexity also imposes a great challenge regarding optimization and systematical testing of transient control strategies in an engine test bed could be both expensive and time consuming.

The objective of this project is to facilitate optimization of transient control strategies. This should be done by identifying appropriate measurement methods for evaluation of transients and by providing models that can be used to optimize strategies off-line.

Measurement methods for evaluation of transients have been tested in several experiments, mainly focusing on emission but also regarding e.g. EGR flow. Applicable instruments for transient emission measurements have been identified and used. However, no method to measure soot emissions cycle resolved has yet been found. Other measurements such as EGR flow and temperatures are believed to have significantly decreased accuracy during transients.

A model for prediction of NOx emissions have been used and complemented with a new approach for soot emission predictions that has been developed in this project. The emission models have been shown to be applicable over a wide range of operating conditions with exception for highly premixed combustion. It has also been shown that models developed for steady state conditions can be used for transients operation.

Contents

1 Introduction

In 1892, a German engineer named Rudolf Diesel patented a new kind of combustion engine. The diesel engine's advantage over other internal combustion engines was, and still is, its efficiency. The engines spreading vary in different markets depending on the geographical position, fuel supply and sometimes tradition. It also varies in different market segments; it is more dominating in high mileage segments where the improved fuel economy surpasses its higher price. The diesel engine is dominating in heavy application such as busses and trucks and its market share in the passenger car segment is steadily increasing, mainly due to increasing fuel price and improved emission. In 2007, 53 % of the sold cars in the European Union were powered by a diesel engine [1].

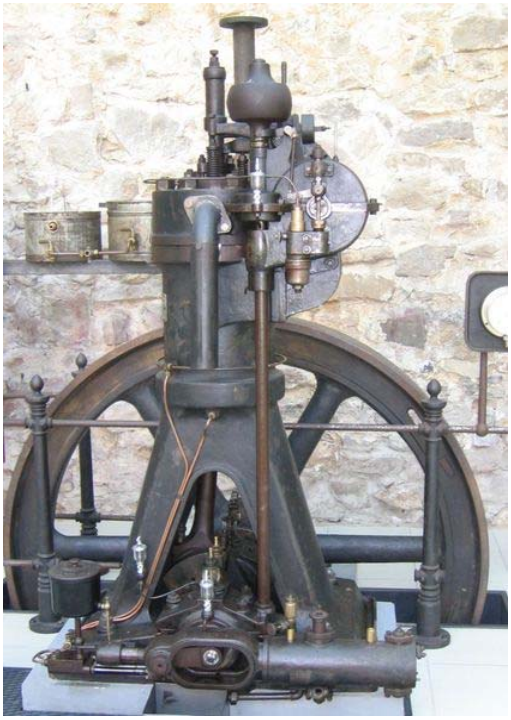

Figure 1 An early diesel engine, [2].

In a diesel engine, the fuel is injected directly into the cylinder during the last part of the compression stroke and the first part of the expansion stroke. The injected fuel mixes with the air in the cylinder and ignites due to the high temperature of the compressed gases in the cylinder. The ignition usually occurs during the initial part of the injection and the fuel that has been injected up to that point combusts rapidly. This part of the combustion is called the premixed combustion period and can be a significant fraction of the total combustion period, typically when the injection duration is short. The fuel that is injected after this point burns as it has evaporated and mixed with air to in combustable proportions after only a short reaction time compared to the initial ignition delay. This combustion period is therefore called diffusion combustion. The combustion process is both turbulent and instationary but a time averaged, conceptual model for the diffusion combustion period has been proposed by Dec ([3]) and this provides a simplified way to describe the process. Dec's model is shown in a schematic in figure 2 together with a picture of a "real" combustion in an optical access engine.

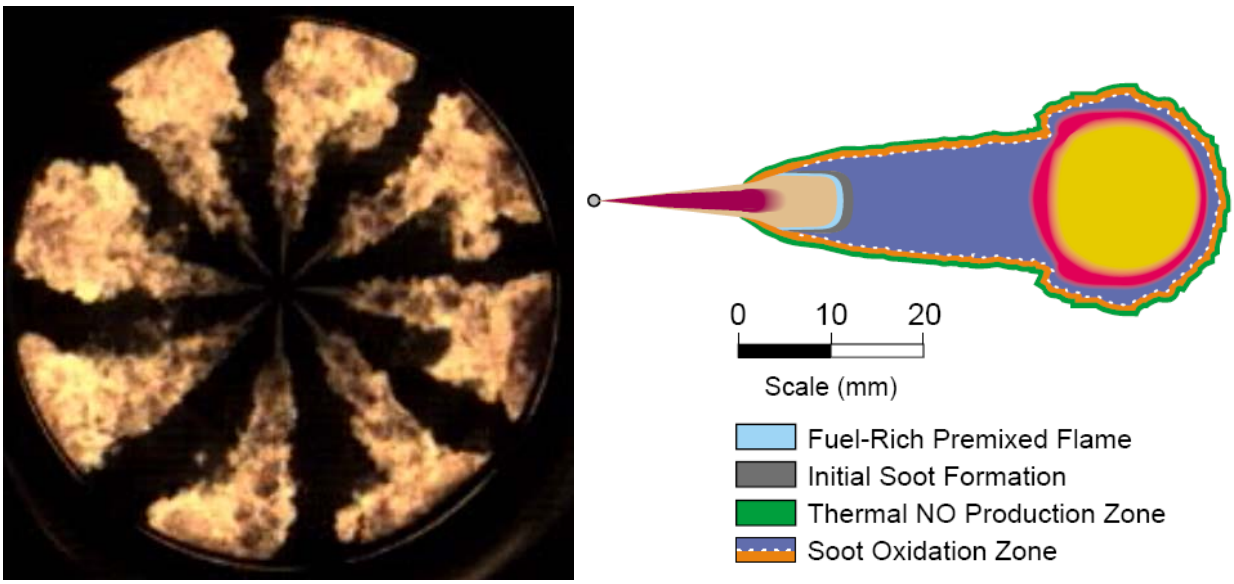

Figure 2 Diesel combustion process, [3], [4]

The disadvantage with diesel combustion, compared to e.g. Otto combustion (normally petrol also called Spark Ignited (SI) combustion), is that it is not homogenous throughout the cylinder, i.e. parts of the combustion takes place with a shortage of oxygen, so called rich conditions. Where there is rich combustion, soot is formed and although most of it is oxidized as the fuel is further mixed with the surrounding air, some of it will remain as the gases are expelled out of the cylinder and through the tailpipe. The regions were soot is formed according to Dec's model is the brown region shown in Figure 2. Soot is emitted from the engine in the form of particles on which water and hydrocarbons are condensated as the exhaust gases are cooled down. These particles are together with other solid and liquid material in the exhaust gases called Particulate Matter (PM).

Particulate matter is a hazard for human's health and to the environment and is together with NOx the main emission from the diesel engine and thereby one of its greatest challenge. Figure 2 also show a green region where most NO is formed; in the flame front where the air/fuel mixture is approximately stoichiometric and the flame is as hottest. NOx is also formed in SI engines but since these are operated without excess air, they can take care of the emissions relatively easy with a three-way catalytic converter. This is not possible in the diesel engine where overall air excess is necessary to achieve acceptable combustion efficiency and soot emissions.

PM-emissions have been shown to increase respiratorical symptoms, decrease lung function and increase use of asthmatic medicine. Increased health care and mortality has also been proved regarding cardiovascular and lung diseases [5].

NOx has been shown to cause increased sensitivity to the respiratory passages [5] and is also the cause of smog. By the influence of sunlight, NOx forms smog together with hydrocarbon emissions.

The maximum allowed quantities of these emissions are limited by the local emission legislations. In Europe, these have been defined by European Union directives in 1992 and tightened in several steps afterwards (Euro 1, Euro 2 etc.). As of 2008, the Euro 5 legislation is coming into effect and the next planned step is in 2013, however the levels for Euro 6 are not fixed yet. The legislated levels are shown in Figure 3 where each marker represents a Euro level (Euro 2 was updated one time and therefore has two markers). It should be noted that since the first Euro level, the maximum allowed PM emissions have decrease by 95 % and NOx with 75%. When the suggested levels for Euro 6 come into effect, the corresponding decrease will be 97 % and 95 % respectively.

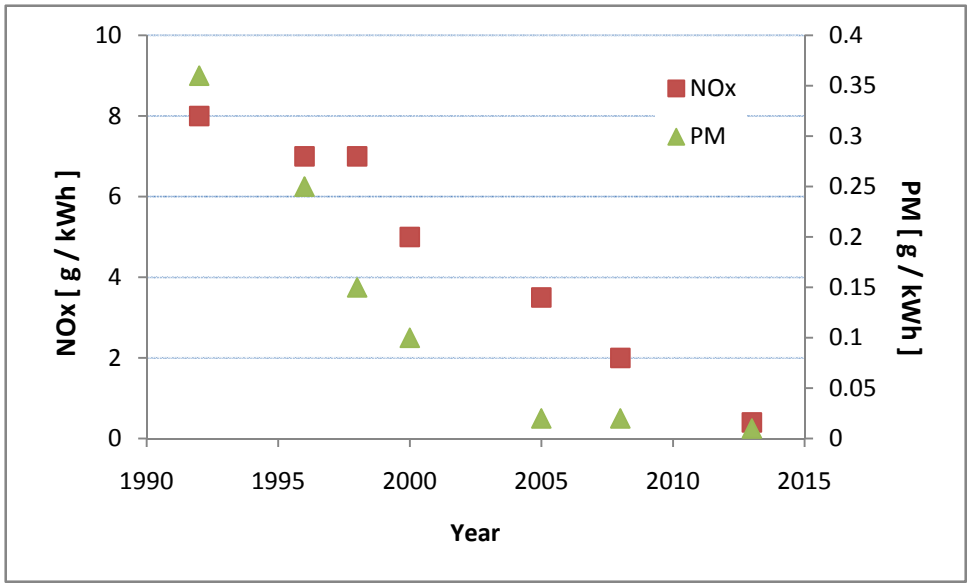

Figure 3 Emission legislation evolution in Europe, [1]

To control that the legislation is met, the engine manufacturers have to certify their engines according to procedures also defined by European Union directives. Before year 2000, the certification procedure only included stationary operation points, i.e. the engine was operated at thirteen defined stationary conditions (% of maximum speed and load) and these were weighted to represent typical engine usage. After the year 2000, since Euro 3, transient engine operation has been included in the certification procedure to better represent real world usage.

The European Transient Cycle (ETC) has been used for Euro 3 to 5 and is shown in Figure 4. This cycle will be replaced by a World Harmonized Transient Cycle (WHTC) for Euro 6. The WHTC has been created to cover typical driving conditions in the EU, USA, Japan and Australia where local certification cycles are used today. The stationary part of Euro 6 will also be harmonized.

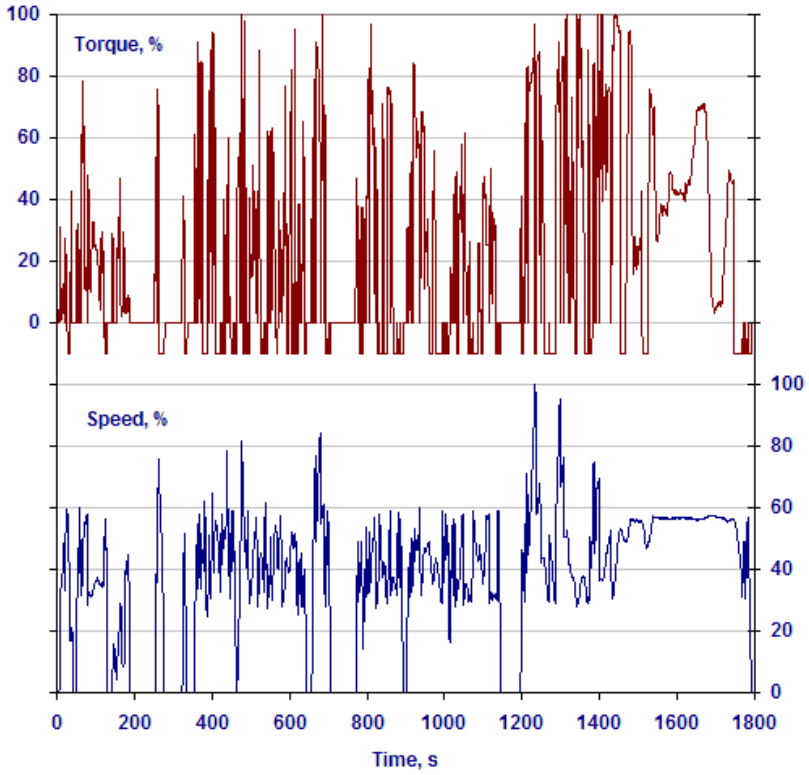

Figure 4 European Transient Cycle, ETC

As can be seen in Figure 4, the ETC cycle is highly varying regarding both load and speed and there are significant consequences when adding this part of the certification to the stationary.

In steady state conditions, different combinations of load and speed correspond to different conditions in the engine regarding the gas flow in the engine's gas exchange circuits and regarding the temperature of all gases, liquids and components. When a transition from one load and speed to another is demanded from the engine, the steady state flows and temperature will not be obtained

directly due the rotational inertia of the turbocharger and the thermal inertia of the components in the engine. The period between when the new load and speed were issued until when the corresponding steady state flows and temperature are reached is what is usually referred to as transient conditions or just transients. In transients, the biggest problem is the rotational inertia of the turbocharger which is the property responsible for the so-called turbo lag when the power demand is increased. When more power is demanded from the engine, the turbine and compressor needs time accelerate its rotational speed and air flow to match the demand.

In an Otto engine, the injected amount of fuel is more or less proportional to the airflow since the engine has to run stoichiometric to make the catalytic converter work properly and therefore the transient power delivery from a turbocharged SI engine is governed by the turbo (after the initial power increase gained by opening the throttle).

A transient in a diesel engine is a bit different; the engine always operates with excess air and when more power is demanded, the excess amount is minimized to allow the injected amount of fuel to increase faster. The engine is then ran at this minimum excess amount of air until the demanded amount of fuel is reached and thereafter the air/fuel ratio will increase again until it reaches the corresponding steady state value.

This period during a power outtake increase (e.g. acceleration), when the air/fuel ratio is lower than the corresponding steady state value, causes increased soot emissions due to the impaired conditions for oxidation. The peak values of the transient soot emission can be more than ten times higher than the corresponding steady state values [6]. An (a perhaps a bit extreme) example of such occurrence can be seen in Figure 5.

Figure 5 Soot can be an issue during acceleration [7]

There are several different measures to decrease the transient soot peaks but transient engine control strategies also has to consider other aspects, mainly engine response (power increase rate) and NOx emissions. Unfortunately the requirements of the different aspect are often contradictory. An effective and widespread way to decrease NOx emission is the use of Exhaust Gas Recirculation (EGR). However, the engine response is dramatically slower when EGR is used under transients and the soot emissions are significantly increased as EGR "steals" energy from the turbine and thereby slows down the boost build up. Another contradiction is the minimum allowed air/fuel ratio allowed during the transient; a lower value means that the fuel injection rate can be increased faster and thereby increases the engine response but at the same time, this means a higher soot emission peak.

The EGR rate and the minimum allowed air/fuel ratio are control parameters that should be optimized as well as VGT strategy (Variable Geometry Turbine) and injection strategy (injection angle, injection pressure and multiple injections).

Even though aftertreatment systems are becoming better, further decrease of the engine out emissions is necessary for future emission legislation levels. In steady state operation, these parameters can be systematically optimized in an engine test bed to obtain the best compromise between soot, NOx and fuel efficiency. For transient operation on the other hand, when not only load and speed has to be considered but also the transient state, systematically testing can be extremely time consuming due to the very high number of combinations of conditions and control settings. Transient control optimization is therefore a great challenge.

2 Project objectives

The aim of this PhD project is to improve the understanding of transient phenomena and to develop tools for transient control optimization. In more concrete terms, the objectives are to be able to:

- measure NOx and soot during transients
- measure transient flow and gas temperatures
- simulate transient turbo performance
- simulate transient EGR flow, temperature and mixing ratios
- simulate NOx and particle formation

Even though the transient cycle has been included in the certification procedure since year 2000, most of the emission measurement techniques that are still used stem from instruments developed for steady state testing. As an effect of this, most instrument have given priority to properties such as measurement -stability and –reproducibility and long service intervals. Very few instruments therefore have the response time necessary to study the cycle to cycle phenomena that occur during transients.

The first part of the project has been mostly about finding emission instruments that are suitable for transient measurements and this has been done by testing both instruments developed for steady state measurements and also some instrument with newer technology developed for transient measurements.

Gas flows such as EGR flow and the air flow into the engine are also difficult to measure with high time resolution and so are most temperatures. The reason for this is also that the established techniques for these measurements are developed for steady state measurements. EGR is usually measured by emission instruments which already have been discussed. Air flow is often measured a bit

upstream from the engine, meaning that e.g. pressure build up after this point must be accounted for separately.

Temperatures are often measured with thermocouples which function by assuming the gas temperature and the response time here is determined by the thermal inertia of the thermocouple. The transient response of a thermocouple can be improved by making it smaller but it cannot be made to small since it would become too sensitive for the rough environment in the engine.

While the two first objectives are all about increasing the understanding and quantifying transient phenomena, the three last objectives are about developing tools for transient control optimization. One way to get around the problem with highly time consuming testing in engine test beds is too develop predictive tools so that all control settings can be optimized by off-line simulations. One version of this solution would be to use somewhat simplified models for shorter computational times and then do the fine tuning in a test bed.

Such predictive tools can be divided into three categories:

Firstly engine performance models. These should be able to predict the behavior of the complete gas exchange system including turbochargers, EGR-circuit etc and how it responds to different control settings during transients. The models in this category are often 1-D models or mean value models.

The second part is prediction of the in-cylinder conditions. The simplest way to models this is to assume that the in-cylinder mixture is homogenous. This strongly simplified approach cannot predict any details about the combustion but can be enough to use in the first category; engine performance models. The most realistic way to model the in-cylinder conditions is with CFD (Computational Fluid Dynamics), where many details in the combustion process can be resolved by dividing the cylinder into a fine mesh of subvolumes. The disadvantage with CFD is that it is very time consuming and that it sometimes can be hard to verify the

details of the combustion since these are difficult to measure. There also exist a number of approaches that lie somewhere between these two approaches regarding the level of details that can be resolved, e.g. 2-zone combustion models and multizone combustion models.

The third and final part is the emission formation calculations. Emission formation rate is calculated with chemical reaction schemes. These schemes occur in literature with a wide range of complexity and they describe how fuel and air is turned into water, carbon dioxide and byproducts via a number of intermediate reactions and species. The most detail schemes include thousands of reactions but sometimes only using a few of them can be useful.

The different models and model categories will be described more thoroughly in the next chapters.

3 Emission formation in diesel engines

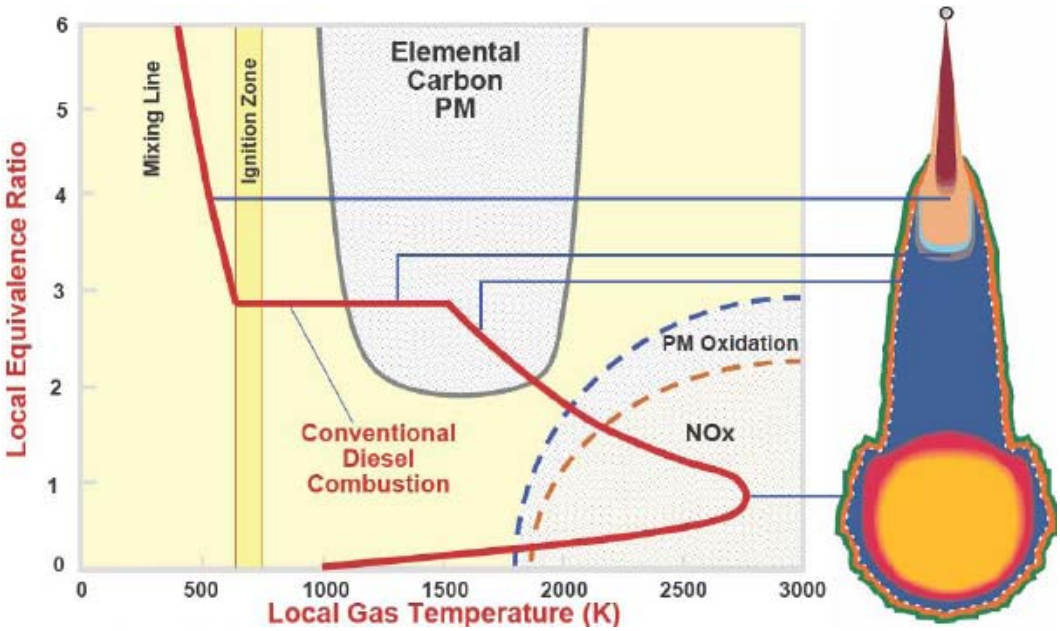

Figure 6 Emission formation in conventional diesel combustion, [8].

Figure 6 shows a so-called phi-T map. In this map, the typical "regions", in terms of temperature and equivalence ratios (phi), for NO formation and soot (PM) formation/oxidation are shown. The figure also contains a "mixing line" which represents the typical path of a fuel package. There are also lines that show where in the phi-T map different sections of the flame typically are.

A phi-T map is commonly used to describe how different combustion concepts affect the emission formation. One important and widely accepted theory shown in such map is that soot is formed in the rich regions of the flame and that it's only formed within a certain temperature interval. HCCI combustion for example avoids soot formation by not having rich regions and the newer concept "Low Temperature Combustion" (LTC) avoids soot formation by moving the "mixing line" to the cold side of the soot formation peninsula.

The figure also shows that NOx formation and soot oxidation occur in the same region, i.e under the same conditions. This is the explanation to why measures to decrease one of the emissions often lead to an increase in the other. This results in the well known soot-NOx trade off curve shown in figure 7.

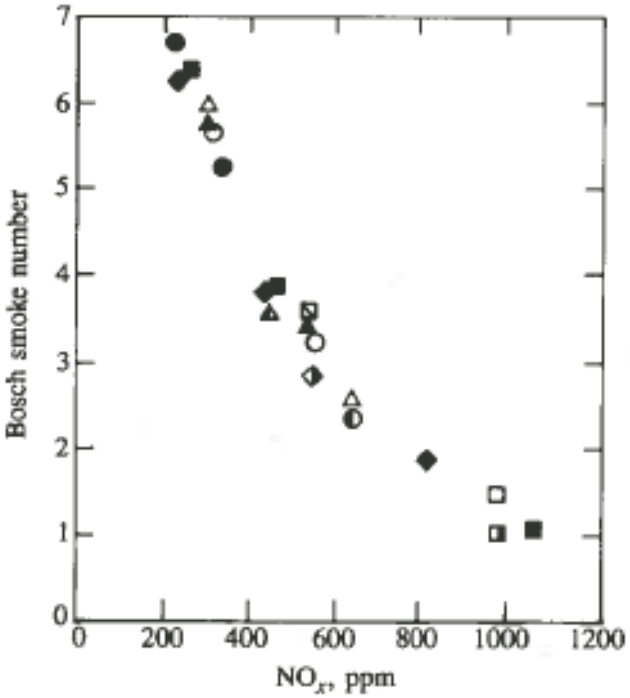

Figure 7 Example of a soot-NOx trade off curve. [9]

3.1 NOx formation

The most important NOx formation mechanism is the Zeldovich mechanism, also called the thermal mechanism since this is responsible for the strong temperature depedence of NOx emissions. The mechanism was proposed by Zeldovich in 1946 [9, 10]:

$$O + N_2 \Leftrightarrow NO + N \qquad (1)$$

$$N + O_2 \Leftrightarrow NO + O \qquad (2)$$

The mechanism was later extended to include a third reaction:

$$N + OH \Leftrightarrow NO + H \qquad (3)$$

As long as the maximum combustion temperature is fairly high (above ~2000 K), the Zeldovich mechanism is dominating the NO production. Otherwise, e.g. when high EGR rates are used or with HCCI combustion, other mechanisms can have significant contribution. Besides the Zeldovich mechanism, there are three other suggested mechanisms [9]:

- The promt (Fenimore) mechanism in which NO is formed from an intermediate specie in the rich zones of the flame
- The nitrous oxide (N2O) mechanism
- NO formation from fuel nitrogen

An automotive diesel engine can typically not avoid high temperature regions in its entire operational range (of load and speed and in transients) and therefore the Zeldovich mechanism is often considered to be dominating.

3.2 Soot formation and oxidation

Soot formation and soot formation modeling is, in several aspects, more complex than NOx formation. One reason is that NOx is formed only via gas-phase reactions while soot formation also includes solid phase reactions. Another reason is that the exact mechanisms are not known and no simple dominating soot formation mechanism have been identified (comparable to the Zeldovich mechanism for NOx formation). However, several reaction schemes and mechanisms have been proposed and some of the most widely accepted are briefly described here:

The precursors for soot formation are formed via the gas phase reaction during fuel pyrolysis. One important precursor is believed to be PAHs (PolyAromatic Hydrocarbons) and the growth process of these precursors appears to involve addition of C_2, C_3 or other small units as, e.g., C_2H_2, acetylene [11].

The reaction step when these gas phase species becomes particles is called nucleation. Several models for this has been proposed and one of the most popular models is the PAH model in which the PAHs start to stick to each other after they have reached a certain size. These PAH clusters then evolve to solid particles [11].

When these particles have been formed they increase in size in what is called the "mass growth process". This process can be divided into three sub-processes; coagulation, surface growth and dehydrogenation. Coagulation starts immediately after the particle formation and can be described as a sticking collision between particles which significantly increases particle mass and decreases particle number without affecting the total particle mass [12]. The surface growth process is when gas phase species such as acetylene and PAHs is adsorbed to the particles surface [11]. In the final stage of soot formation, the particles are dehydrogenated to progressively more graphitic carbon material. At the same time, the number of active sites on the particle for surface growth is reduced and therefore the dehydrogenation leads to the formation of chain like structures [11].

Simultaneously as the soot formation processes and in many cases until the gases are emitted from the cylinder, the soot oxidation process is taking place. The main oxidating reactants are OH under fuel rich conditions and O_2 under fuel lean conditions [11].

3.3 Emission reduction

The trade off relationship between NOx and soot (Figure 6) is fortunately only fixed for a specific engine and ways to reduce emissions has continuously moved this trade-off curve towards origo to meet new legislations (Figure 3). New combustion concept such as HCCI, PCCI etc. can break the trade off by altering the mixing and ignition parts of the combustion. However, conventional diesel combustion is still dominating and the greatest contribution to the emission reduction comes from component development. One clear trend over the years has been to increase the injection pressure and thereby improve the mixing and reduce the rich regions that cause soot formation. Exhaust Gas Recirculation (EGR) had its break through for Euro 4. The use of EGR decreases the maximum combustion temperature and thereby the NOx formation. Lower combustion temperature means worse soot oxidation but this can be compensated for by increasing the boost pressure and thereby the air/fuel ratio or by increasing the injection pressure further.

Since the Euro 4 emission level, many engine manufacturers have been forced to equip the engines with aftertreatment systems since they were no longer able to sufficiently reduce the engine-out emissions. The most common aftertreatment systems are Particulate Traps and Selective Catalytic Reduction (SCR) where NOx is reduced with a reductant e.g. ammonia. However, the engine-out emissions still need to be reduced and controlled. An SCR aftertreatment system only reduces 70-95% so the engine-out emissions can still not be too high. Another factor is the cost of the reductant that has to be added. For all aftertreatment systems, size and service interval are also strong arguments to reduce the engine out emissions.

4 Diesel combustion modeling

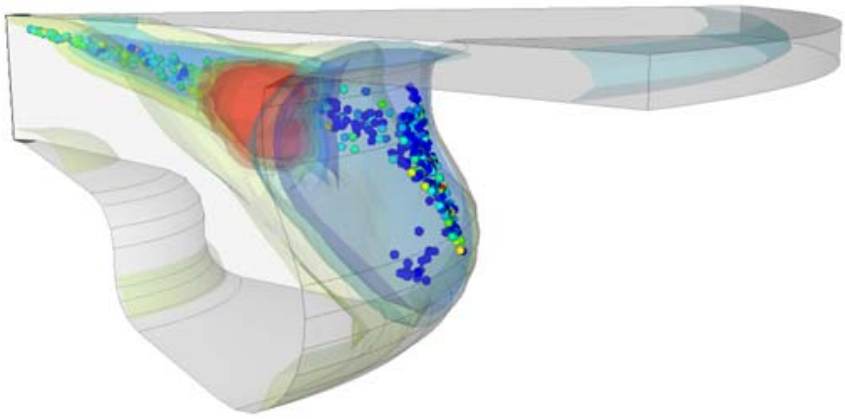

Figure 7 CFD Modeling of the diesel combustion process [12]

Since the combustion process in a diesel engine is very complex, the only possibility to model it realistically is by using CFD coupled to a chemical reaction model. A realistic model has to be able to describe in-cylinder flow induced during the intake stroke with properties such as swirl and tumble. It has to be able to predict how the fuel spray breaks up, evaporates and mixes with the air in the cylinder, how the first reactions start and the mixture auto-ignites and thereafter the diffusion combustion. It also has to be able to predict the in-cylinder flow after combustion and heat transfer to the cylinder walls and roof and to the piston. Many of these processes are difficult to predict separately and are extremely challenging combined.

In CFD combustion modeling's, the combustion chamber is divided into sub volumes. The number of sub volumes that are used ranges from thousands up to three orders of magnitude more. The greatest advantage over other models is the high level of detail that can be resolved. If a model has been thoroughly validated,

it can increase understanding of the combustion process and the model can be used to predict the influence of e.g. injector properties and piston bowl design. It can also show where the greatest contribution to the emission origin and how it is avoided.

The formation of soot and NO emission can be predicted via chemical kinetics reaction schemes that often are extensive. These schemes describes how fuel and air are converted to carbon dioxide and water via thousands of reactions and hundreds of intermediate species and are also used to predict auto-ignition and heat release rate. NOx formation can be included in the schemes while soot formation can only be partly included since soot formation also consist of solid matter reactions and not only gaseous.

Some examples of soot models where these complex gas phase chemical reaction schemes are used together with particle growth models in CFD models are [13-16].

The greatest disadvantage of using these complex models is the computational time. Depending on the number of sub volumes in the model, the complexity of the model, computer capacity, etc., computing one engine cycle require from a couple of hours up to days. If one considers engine transients; one large load transient in a heavy duty engine has a duration of over 50 cycles and to find optimum control setting for this transient, hundreds of combinations of settings would have to be simulated. In practice, this means that it isn't feasible to use these models for transient control optimization, i.e. simplified models are needed for that application.

4.1 Simplified diesel emission modeling

To decrease the computational time needed for emission predictions, the models can be simplified in three aspects: how the combustion process is modeled, the chemical reaction schemes and the models that describes the emission formation processes.

4.2 Simplified combustion modeling

Simplifications of the combustion process can be found in many different degrees in literature. One common simplification that significantly reduces the complexity of the model is to disregard the spatial resolution, i.e. use 0-D models. The most common 0-D models are:

- Homogenous in-cylinder conditions [17]
- Two-zone combustion models [18-20]: One zone with reactants and one zone with products.
- Multizone combustion models [21-24]: One zone with reactants and one zone with products for each time step after the start of combustion.

The two-zone approach is considered to be a fairly accurate way to describe SI combustion [10] since the fuel/air mixture is homogenous throughout the cylinder and the flamefront propagates outwards from the spark-plug in the center of the cylinder with products behind it and reactants in front of it. The two-zone approach is however less straight forward when it comes to diesel combustion due to inhomogenous in-cylinder conditions and a much less regular combustion process. The common way to solve this is to assume that the combustion takes place at stoichiometric conditions and that the combustion products are then gradually mixed with the excess air in the cylinder. Thus, the in cylinder mixture becomes homogenous before the exhaust valves open [18, 20].

The main drawback of using the two-zone model for diesel combustion modeling is that the maximum temperature is underestimated since the temperature in the

burned zone at every instant is an average of all burning and previously burned elements. This underestimation has significant impact on the highly temperature dependent NOx formation process.

To better imitate the real combustion process, multizone models have been developed. In these models, the combustion process is divided into discrete time steps and a new zone with combustion products is formed for each one. The temperature and the mixing processes are still averaged but to a lower extent. The in-cylinder temperatures with the different models are shown in Figure 8.

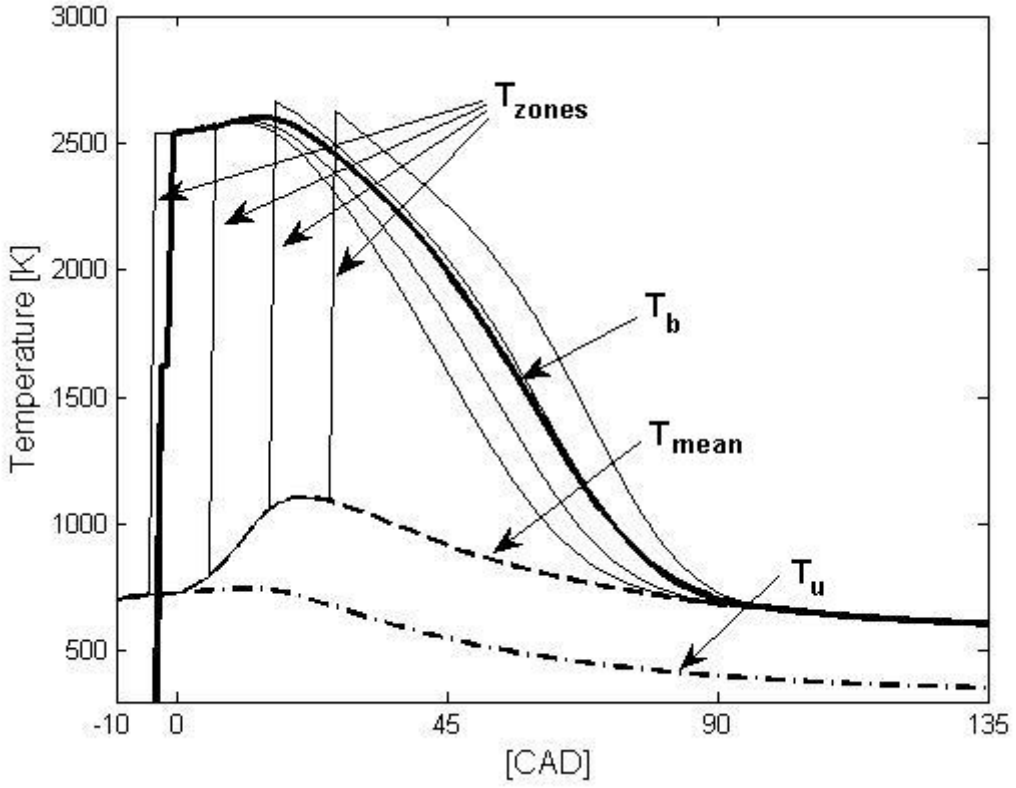

Figure 8 In-cylinder temperatures. T_{mean} is the homogenous temperature. T_u is the temperature in the unburned zone, i.e. the zone containing the reactants in a two-zone model. T_b is the burned zone, i.e. the zone containing the products in a two-zone model. T_{zone} is the temperature in the product zones in a multizone model. In this case four zones are used but normally one zone per degree combustion duration is used, i.e. the number of zones at the end of the combustion is typically around 50.

4.3 Simplified chemical reaction schemes

As previously mentioned, the combustion chemistry in a diesel flame is very complex with hundreds of species and thousands of intermediate reactions. On the lean side of the flame, where the combustion is almost completed, the chemistry is dominated by only a few species and is thereby much simpler to model. The ten species with highest concentration are; CO_2, CO, H_2O, H_2, O_2, N_2, H, O, NO, and OH [10, 21]. As the local changes in temperature and air supply are slow on the lean side of the flame unlike in the rich and stoichiometric sides of the flame, the concentration of these species can be assumed to equal the equilibrium concentrations. The fractions of the different species are found with carbon-, hydrogen-, oxygen- and nitrogen-balance and by finding the equilibrium balance for the following reactions:

$$CO + H_2O \Leftrightarrow H_2 + CO_2 \quad (4)$$

$$CO + \tfrac{1}{2} O_2 \Leftrightarrow CO_2 \quad (5)$$

$$\tfrac{1}{2} O_2 \Leftrightarrow O \quad (6)$$

$$\tfrac{1}{2} H_2 \Leftrightarrow H \quad (7)$$

$$OH + O \Leftrightarrow O_2 + H \quad (8)$$

$$N_2 + O_2 \Leftrightarrow NO + NO \quad (9)$$

This combustion chemistry can be used to predict processes on the lean side of the flame such as NO_x formation and soot surface oxidation.

4.4 Simplified emission modeling

Simplified emission modeling can be divided into three categories:

- Phenomenological models
- Semi-empirical models
- Statistical (cycle resolved) models

4.4.1 Phenomenological models

A phenomenological model is one which relates empirical observations of phenomena to each other, in a way which is consistent with fundamental theory, but is not directly derived from theory. This category of modeling is a way to deal with the complexity of soot formation where important and representative species and mechanisms for the soot formation process are modeled. One example of a phenomenological model was proposed by Fusco et al in 1994 [17]. Each part of the soot formation and oxidation process was represented by one equation reaction as illustrated in Figure 9.

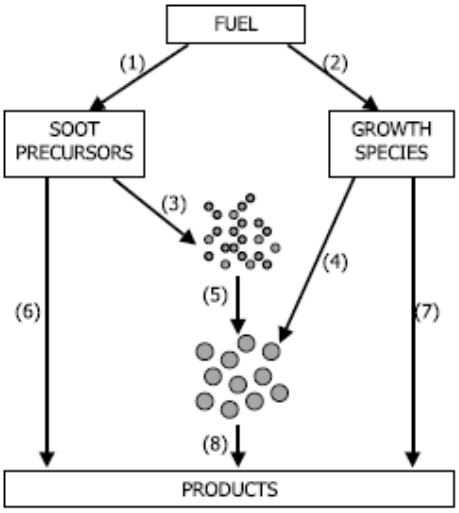

Figure 9 Illustration of Fusco et al's Soot model [17]. Schematic figure from [25]

The reactions can be summarized in four equations:

$$\frac{d[R]}{dt} = v_1 k_1 [Fuel] - k_3 [R][O_2] - k_5 [R] \quad (4)$$

$$\frac{d[C_2H_2]}{dt} = v_2 k_2 [Fuel] - k_4 [C_2H_2][O_2] - k_6 [C_2H_2]\sqrt{A_{soot}} \quad (5)$$

$$\frac{d(f_v)}{dt} = \left(k_5 [R] - k_6 [C_2H_2]\sqrt{A_{soot}} - \frac{6 m_{soot}}{\rho_{soot} D_{soot}} \dot{R}_{NSC}\right) \rho_{soot} M_{soot} \quad (6)$$

$$\frac{d(f_N)}{dt} = \left(k5[R] - k_8 \sqrt{T} \sqrt[6]{f_v} \sqrt[\frac{11}{6}]{f_N}\right) N_A \quad (7)$$

$[R]$ and $[C_2H_2]$ are the concentrations of soot precursor species and growth specie (acetylene). v_i and k_i are the stoichiometric coefficient and reaction rate coefficients. f_v and f_N are soot volume fractions and particle number concentration. m_{soot}, M_{soot}, ρ_{soot}, D_{soot} and A_{soot} are the soot- mass, molar mass, density, average diameter and surface area concentration (cm2/cm3). N_A is Avogrado's number. $\dot{R}_{NSC}$ is the soot oxidation rate calculated with the Nagle and Strickland-Constable (NSC) model:

$$\dot{R}_{NSC} = \left[\left(\frac{k_A p_{O_2}}{1 + k_A p_{O_2}}\right) X_A + k_B p_{O_2} (1 - X_A)\right] \quad (8)$$

Where R_{NSC} is the oxidation rate [mol C-atoms/(cm2*s)], k_A k_B and k_Z, as well as k_T which is used in the next equation, are temperature dependent rate functions, p_{O2} is the partial pressure of oxygen. The molar fraction of O_2 was approximated by the equilibrium molar fraction, which is already calculated for the NO formation rate. x_A is the fraction of soot with a more reactive surface site.

x_A is calculated with the following equation:

$$X_A = \left(1 + {}^{k_T}\!/_{k_B p_{O_2}}\right)^{-1} \quad (9)$$

When Fusco et al presented this model they used average in cylinder conditions [18], but it has also been used together with CFD (Computational Fluid Dynamics) modeled in cylinder conditions [three]. Extended versions of the model has also been used, e.g. [26, 27] and there are also alternative models proposed, e.g. [28, 29].

Another example of phenomenological models is models where different reaction rates are curve fitted to other parameters such as temperature. For example, the complex calculations for soot formation rate that are shown in Figure 6 on a phi-T map have been curve fitted as a function of phi (fuel/air ratio) and temperatures and used in CFD [8].

A common method to predict NO formation is to assume that the thermal NO formation is dominating and that the thermal (Zeldovich) mechanism can be used to predict the total NO formation. From the extended Zeldovich mechanism, eq.1-3, the rate of NO formation can then be written as:

$$\frac{d[NO]}{dt} = k_1^+[O][N_2] + k_2^+[N][O_2] + k_3^+[N][OH]$$

$$-k_1^-[NO][N] - k_2^-[NO][O] - k_3^-[NO][H] \quad (10)$$

Where [ ] denotes concentration of the different species and k_i denotes the forward and reversed rate coefficients. The rate constants are strongly temperature dependent and can be found in e.g. [10]

The concentration of the species included in the equation, and thereby the formation rate, can be obtained if complex gas phase reaction schemes are used. Examples can be found in in-cylinder CFD combustion and emission models, e.g. [13, 14]. If reaction schemes are not used, the “equilibrium assumption”, [10], can be used since most NO is formed on the lean side of the flame. This approach is used by e.g. [21] and leads to the following simplified expression:

$$\frac{d[NO]}{dt} = \frac{2R_1\left\{1-\left({[NO]}/{[NO]_e}\right)^2\right\}}{1+\left({[NO]}/{[NO]_e}\right){R_1}/{(R_2+R_3)}} \quad (11)$$

Where $[\ ]_e$ denotes equilibrium concentration and

$$R_1 = k_1^+[O]_e[N_2]_e = k_1^-[NO]_e[N]_e \quad (12)$$

$$R_2 = k_2^+[N]_e[O_2]_e = k_2^-[NO]_e[O]_e \quad (13)$$

$$R_3 = k_3^+[N]_e[OH]_e = k_3^-[NO]_e[H]_e \quad (14)$$

4.4.2 Semi-empirical models

Semi-empirical models can be described as a further simplification of the phenomenological models. The most popular example is the two-step Hiroyasu model which has was presented in 1983 [30] with one reaction for soot formation and one for oxidation:

$$\left.\frac{dm_{soot}}{dt}\right|_{form} = A_f m_{fuel} p^{0.5} \exp\left(\frac{E_f}{RT}\right) \quad (15)$$

$$\left.\frac{dm_{soot}}{dt}\right|_{oxid} = A_o m_{soot} X_{0_2} p^{1.8} \exp\left(\frac{E_o}{RT}\right) \quad (16)$$

Where m_{soot} and m_{fuel} are the mass of soot and fuel vapor. A_f and A_o are the pre-exponential constants for soot formation and soot oxidation respectively and they are adjusted empirically. E_f and E_o are the activation energies and are also adjusted empirically. X_{0_2} is the oxygen molar fraction. p, T and R are in-cylinder pressure and temperature and the gas constant.

This model has been widely used, thanks to its simplicity. A disadvantage is that it only is valid in a narrow range of operating conditions. The model can be used with one-, two-, and multizone models as well as with CFD models [8, 18, 24 and 28].

4.4.3 Statistical models

Statistical models ([22 and 31-33]) are usually cycle resolved “black box” models where the emissions are predicted by curve-fitting cycle averaged and/or cycle characteristic data to emissions. This type of modeling is the fastest and it doesn’t require any deeper understanding of the underlying mechanisms. The disadvantages are that high accuracy usually can’t be obtained over wide ranges of operating conditions and that they are unreliable for extrapolation.

Statistical modeling could be a useful tool for rough off-line optimization of transient control strategies thanks to the simplicity of the models and the short computational time. The problem is that more or less all measurements are somewhat delayed and filtered or smoothened. Pure delay can often be identified and corrected for rather easy but the filtering caused by the instruments rise times is harder to identify and correct for. This makes it more difficult to identify what parameters that are the most important and their cause-effect relationship. To illustrate this, an artificial signal and a filtered version of the same signal is shown in the upper part of Figure 10. The floating average filter that is used here represents an instrument rise time of ~0.7 second. A reasonable example for, e.g., the soot measurements.

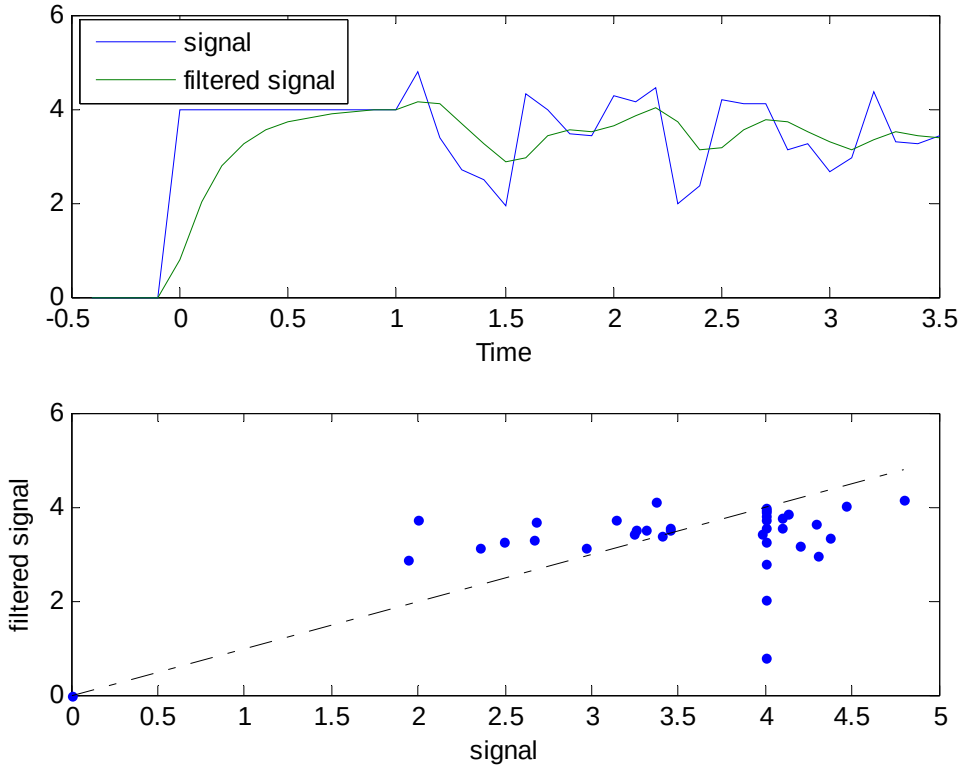

Figure 10 Effects of instrument rise time on statistical models.

The lower part of Figure 10 shows the correlation between the signal and its filtered version and shows why it is difficult to create statistical models for transient operation, especially if the instruments rise time is unknown. The case is often that both cause- and effect parameters have significant (and different) filtering.

It would be an option to develop the models during stationary operation where the instruments rise times isn't a problem. However, the extreme conditions that occur during transients (extremely low air/fuel ratio) are difficult to achieve in stationary operation.

5 Advantages and disadvantages of different emission model categories -Motivation for chosen models

The type of models used for emission predictions in this project was chosen by evaluating the advantages and disadvantages of the different model categories. The CFD models with complex chemistry and particle growth models were eliminated at an early stage due to computational cost. The cycle resolved models on the other hand have a very low computational cost but do not give any physical understanding of the underlying processes and there is also the practical problem with establishing cause-effect relationships due to the rise times of different measurement methods. The model category that was chosen for this project was therefore the simplified physical model category.

One specific work that influenced the model development in this project was Egnell's NOx models [21]. In this model a multizone approach is used to model the combustion process, the equilibrium assumption is used to predict the composition of different species in the cylinder and the NO formation rate is calculated with the extended Zeldovich mechanism.

From this NOx model, a new approach for soot predictions was developed. Soot oxidation on the lean side of the flame is believed to be dominated by O_2 surface oxidation [11] and can thus be predicted by using the Nagle and Strickland-Constable model in the framework of the NOx model, i.e. a multizone combustion model and equilibrium combustion chemistry.

Since the multizone model only describes the products of combustion, i.e. starting in the stoichiometric and lean regions of the combustion, the soot formation and OH oxidation processes cannot be included since these occurs at rich conditions.

To get around that problem, a new approach was attempted based on two observations; firstly in a phi-T map, e.g. Figure 6, it can be seen that NOx formation and soot oxidation occur under the same conditions, i.e. high

temperature and with available oxygen. The second observation is the NOx-soot trade off curve, which clearly shows that operating conditions that result in high NOx emissions also result in low soot emissions and vice versa. The conclusion of these observations is that since it is possible to predict NOx emissions with the multizone model it should be possible to predict soot emissions as well.

A secondary product of that conclusion is that the variations in the soot formation process on the rich side of the flame are less significant for the emissions than the variations in the oxidation process on the lean side of the flame. Thereby, a good estimation of the emitted soot should be found if a "typical" soot formation process for the specific engine can be found and if the oxidation process is described correctly.

In this approach it was assumed that the typical soot formation process for the specific engine could be represented as a typical fraction of fuel, with a typical particle diameter, surviving through the flame and to the stoichiometric and lean sides where the multizone model and soot oxidation model are valid.

The typical fraction and diameter for the soot model was found together with typical mixing rate and typical combustion air/fuel ratio for the multizone model by running an error minimization script for the models over a wide range of steady state conditions.

One of the fundamental assumptions in the multizone approach is that the combustion takes place in a developed flame and as a consequence, the accuracy of the model decreases when significant part of the combustion is premixed.

More details of the models are found in the articles in the appendix.

6 Measuring and evaluating transient operation

As described in the introduction section, measuring and evaluating transient operation is in most aspect more difficult compared to stationary operation as it demands information with high time resolution from instruments and measurement methods that were developed for stability, repeatability and durability. The extra precautions and data processing that is necessary to evaluate transient operation will be described in this section.

6.1 Gas exchange system measurements

The performance of the gas exchange system, including the intake- and exhaust-systems and the EGR-circuit, is a very important factor during engine transients and is therefore very important to be able to measure. The performance parameters that are most interesting to evaluate are intake airflow and EGR rate. They are two of the most important parameters for the in-cylinder conditions and are therefore essential as inputs for emission predictions.

6.1.1 Transient EGR measurements

In steady state conditions, EGR rate is typically measured by comparing the CO_2 fraction in the intake with the exhaust concentration but since CO_2 is measured with a conventional instrument, this cannot be used during the transients. Instead, the EGR rate was estimated from air based volumetric efficiency (only fresh air flow is included) via a steady state correlation. This correlation origin from a wide range of operating conditions and is shown in Figure 11.

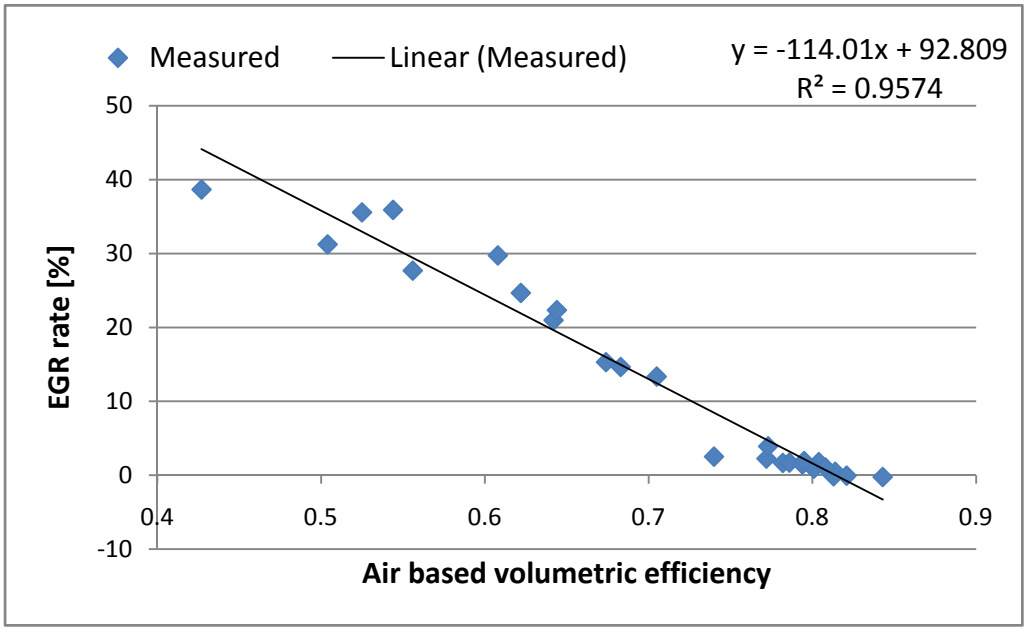

Figure 11 Steady state correlation between air based volumetric efficiency and EGR rate for a wide range of operating conditions

As can be seen in Figure 11, the maximum measured volumetric efficiency is only 0.85. Since the volumetric efficiency is calculated from the swept volume, 100 % efficiency will not be achieved as the intake valves are closed somewhat later than the bottom dead position of the piston. A few percent is also lost due to residual gases in the cylinder, i.e. internal EGR. Variations in internal EGR rate are what cause the errors in the external EGR estimations in the figure and when the estimation is used during transients.

6.1.2 Transient air flow and air/fuel ratio measurements

Since the airflow to the engine is measured before its compressors, there will be a measurement error when the engine is operating transient. This is due to accumulation effects in the intake system during pressure build up. This can corrected for with the following equation:

$$\dot{m}_{corrected} = \dot{m}_{measured} - \frac{V}{R}\frac{\Delta\left(\frac{P}{T}\right)}{\Delta t} \qquad (17)$$

This correction should be done for all subvolumes in the engine's intake system. P, V, R and T are pressure, volume, gas constant and temperature.

To get the correct global air/fuel ratio in the cylinder, the excess air in the EGR also has to be accounted for. These two corrections have significant impact on the estimated air/fuel ratio. Air/fuel ratio was also measured with a wideband unit. However, this also has to be corrected for the air in the EGR.

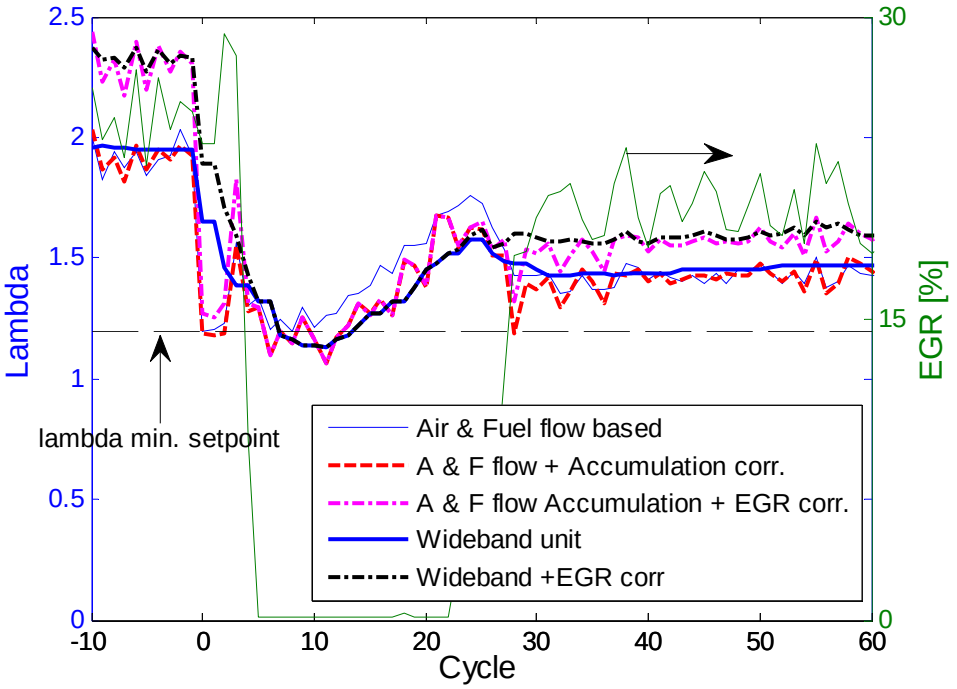

Figure 12 Correction of the estimated air/fuel ratio

6.2 Emission measurements

6.2.1 NOx measurements

In stationary operation conditions, NOx is measured with a ECO Physics CLD 700 chemiluminescence detector. This instrument measures the total of NO and NO_2 measurements but since it has a rise time in the order of 20 seconds it is not useful for transient evaluation. For that application, a Cambustion fNOx400 Fast CLD chemiluminescence detector was used instead. This instrument has a rise time of 4 milliseconds but only measures NO. That is however an acceptable compromise since significant NO_2/NO_x ratios only occurs at high global air/fuel ratios and thus typically not under transient conditions [10].

6.2.2 Soot measurements

Particulate Matter (PM) and soot has been measured in a number of aspects in this project; PM mass concentration [mg/m3], opacity (%), Filter Smoke Number (FSN), particle number concentration [N/cm^3] and size distribution. The different measurement methods has been evaluated and compared [34] and it was concluded that a good characterization of the PM emissions can be achieved if some kind of mass related measurements are performed as well as some size distribution related measurement. Mass related measurements are besides PM mass concentration also opacity and FSN. The most repeatable measurements have been found to be FSN. However, FSN has to be averaged for about 30 seconds and are thereby not useful during transients. Therefore opacity was used for transient measurements instead. Opacity is a bit less stable since it can be affected by liquid PM, humidity and light absorbing species in the exhaust, but it has a rise time of less than one second.

Size distribution measurements and particle number concentration measurements can provide very detailed information about the emitted PM. One of the reasons why these types of instrument have gained popularity recently is that researchers have found correlations between human health and particle number concentrations [5]. It is believed that the reductions in PM-mass emissions have been accomplished by decreasing the average particle mass and not the number of particles. The next emission legislation level, Euro 6, will also include particle number measurements.

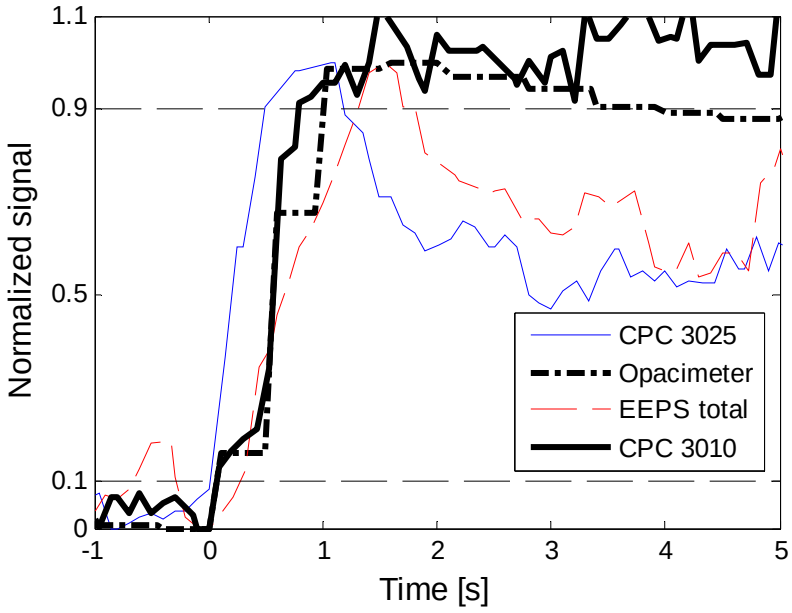

Figure 13 Rise time evaluation for PM instruments

The rise times for the different instruments are showed in Figure 13. This was tested by decreasing the air/fuel ratio significantly from one cycle to the other. In this figure, normalized opacity and particle number measurements in three different size ranges are shown. The particle counters CPC 3025 and CPC 3010 measured the total number of particles larger than 3 and 50 nm respectively. The size distribution measured with the EEPS was integrated and shows the total number of particles larger than 6 nm in the figure. It can be seen in the figure that

the concentration of larger particles correlates better with opacity (and thereby PM mass) than when smaller particles also are included.

The CPC 3025 was chosen to measure particle number concentrations during transients since it is the fastest instrument. It was equipped with a Particle Size Selector so that it only measured particles larger than 20 nm, i.e. to comply with the proposed Euro 6 legislation.

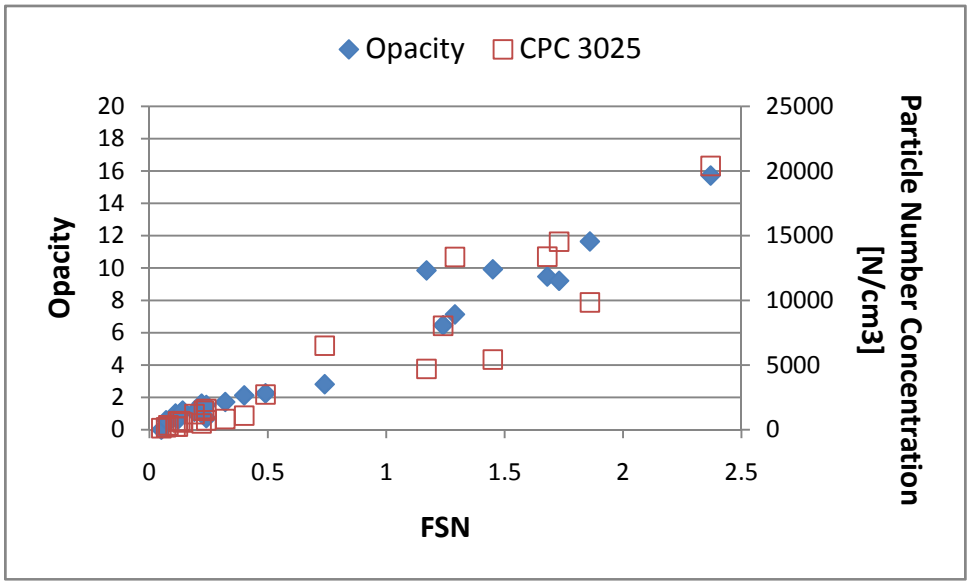

Figure 14 Correlation between PM-measurement methods

Figure 14 shows opacity and particle number concentration, vs. FSN. It shows that Opacity and FSN correlates very well while there are some spread when particle number concentration and FSN is compared, probably due to particle size variations. This data comes from a wide range of steady state operating conditions and curve-fitted linear trendlines was later used to correlate transient measurements to steady state and to estimate size changes during the transients. An example is shown in Figure 15.

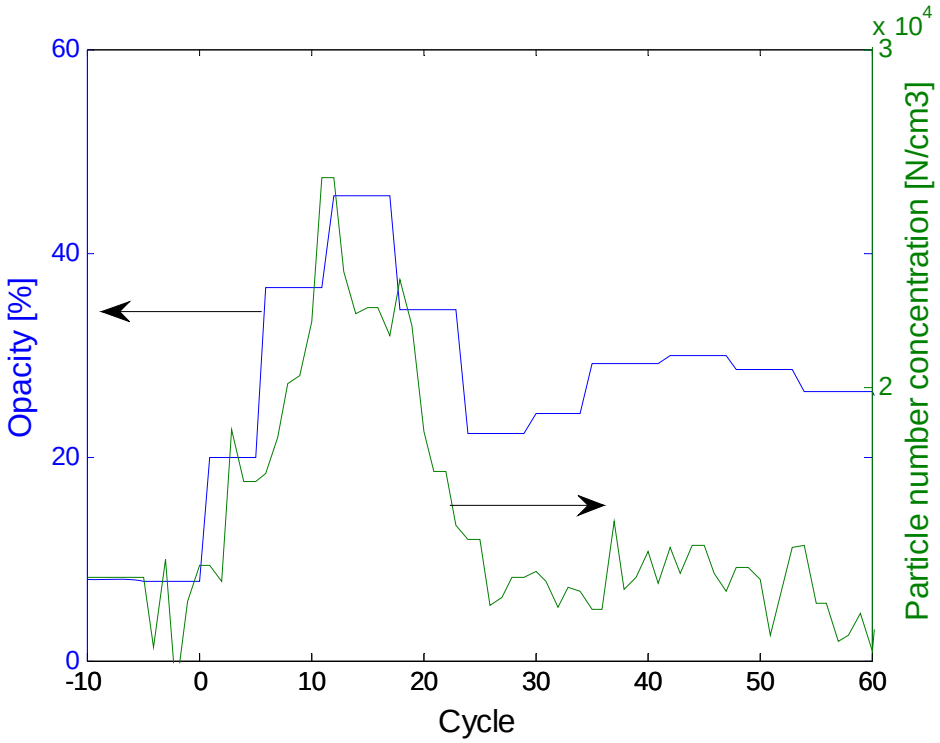

Figure 15 Variations in mass-averaged particle diameter during a transient can be estimated by comparing opacity and particle number measurements.

Figure 15 shows how measured opacity and particle number concentration correlates during a transient. From this correlation, variations in the averaged size of the emitted particles can be estimated. The ratio between opacity and particle number concentration about three times larger after cycle 20 than before. If the mass per particle is increased three times, that corresponds to a diameter increase of ~50 %.

This method for estimation of how the average particle size varies can be used as a step in the validation of soot prediction models.

6.3 Post processing emission predictions

As described, most instruments, and especially soot instruments (figure 13), have significant rise times. This rise time is often caused by internal volumes in the instruments and the result is an averaging/filtering effect. Some averaging also occurs before the exhaust gases reaches the instruments, as gases from different cylinders and cycles are mixed with each other. Since the measurements are not cycle-resolved, some post processing is necessary to make the predicted emission comparable.

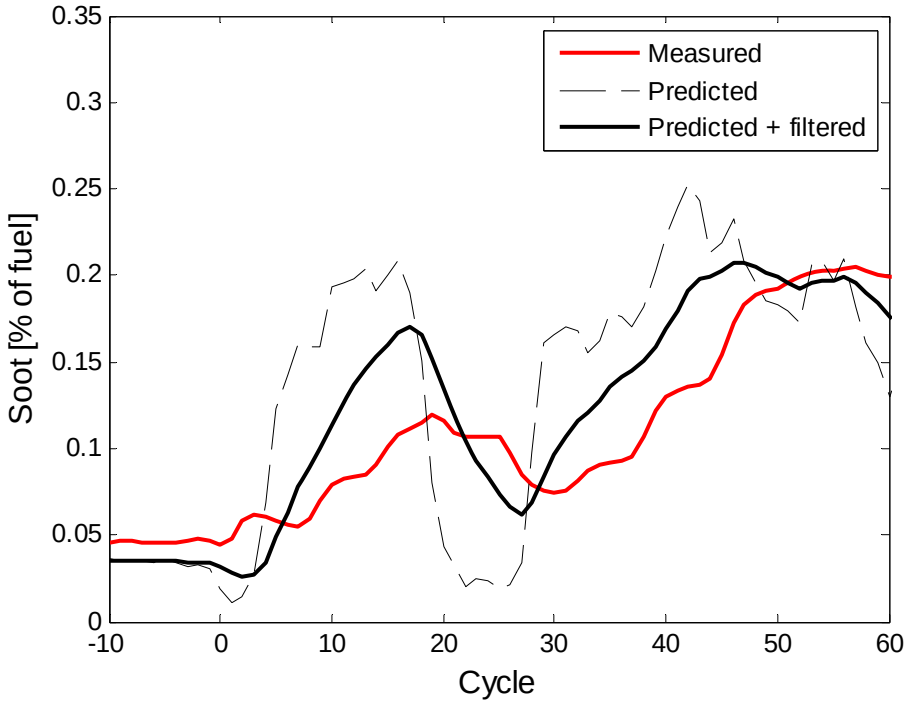

Figure 15 Post processing of predicted soot emissions to imitate exhaust system and instrument averaging and to decrease effects of noisy input data.

Figure 15 shows the predicted soot emissions with and without an averaging filter together with the measurements. The strength of the necessary filtering depends on the instrument to which the predictions are compared. Noisy input data can also increase the need for filtering.

7 Introduction to papers and key results

This section contains very brief summaries of the papers and some of the key results presented in them. The lessons learned from each paper have been carried on to the next one and the long terms goal has been to fulfill the project objectives:

- measure NOx and soot during transients
- measure transient flow and gas temperatures
- simulate transient turbo performance
- simulate transient EGR flow, temperature and mixing ratios
- simulate NOx and particle formation

7.1 Paper 1," Evaluation of Techniques for Transient PM-measurements"

As the title reveals, paper 1 presents an evaluation of different PM instruments regarding their suitability for transient measurements. The tested instruments were a TEOM and an opacimeter for PM-mass and two CPCs and an EEPS for particle number concentration and size distribution. The tests were conducted on a single-cylinder research engine. The most important conclusion from this paper was that the measurements with the highest time resolution were achieved by one of the CPC and the opacimeter, with rise times just below 1 second (see Figure 13). It was also found that the proportionality between PM mass and particle number concentrations vary, mainly due to variations in particle size distribution and that these variations can be decreased if the very smallest particles are disregarded.

7.2 Paper 2, "Predictions and Measurements of Transient NO Emissions for a Two-stage Turbocharged HD Diesel Engine with EGR"

In paper 2, an engine load transient was evaluated with different control strategies, or more specifically, with different EGR rates during the first part of the load increase. The tested heavy duty engine was equipped with a two-stage turbocharging system and a high pressure EGR route. The aim was to predict the engine behavior with the different strategies with a 1-D model and to couple that model to a multizone NO prediction model. The objectives that were focused on in this paper were transient NOx measurements and simulation of transient turbo performance, EGR flow and NOx formation.

The main conclusion were that the multizone NOx model predicted the emissions well and that this model easily could be coupled to the 1-D model without slowing it down significantly. However, due to the high pressure levels in this engine, it is difficult predict the EGR flow in the high pressure route and this has significant influence on the NOx predictions. In this experiment the EGR rate was measured by measuring the NO in the intake and in the exhaust. Examples of results are shown in Figure 16.

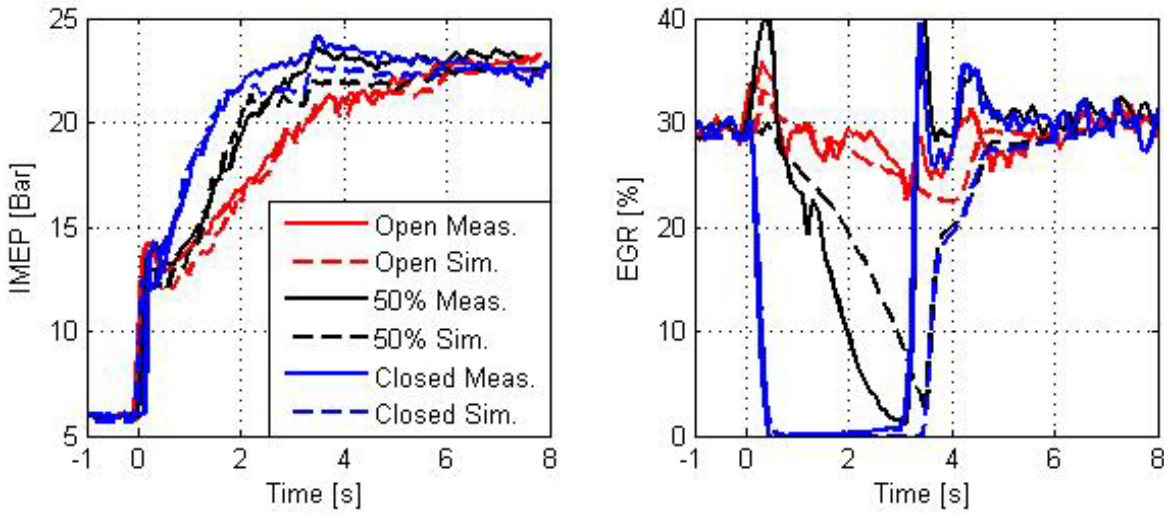

Figure 16 Predicted and measured IMEP and EGR rate with three different EGR-valve settings during the initial part of a transient.

7.3 Paper 3, "Fast Physical Prediction of NO and Soot in Diesel Engines"

In this paper the multizone model used for NOx predictions was extended to include soot oxidation and by strongly simplifying the soot formation process, the soot emissions could be estimated. The model was developed with constant parameters over the entire operational range of the engine and the general agreement was high considering the widely spread operating conditions. The predicted in-cylinder emissions during one engine cycle are shown in figure 17.

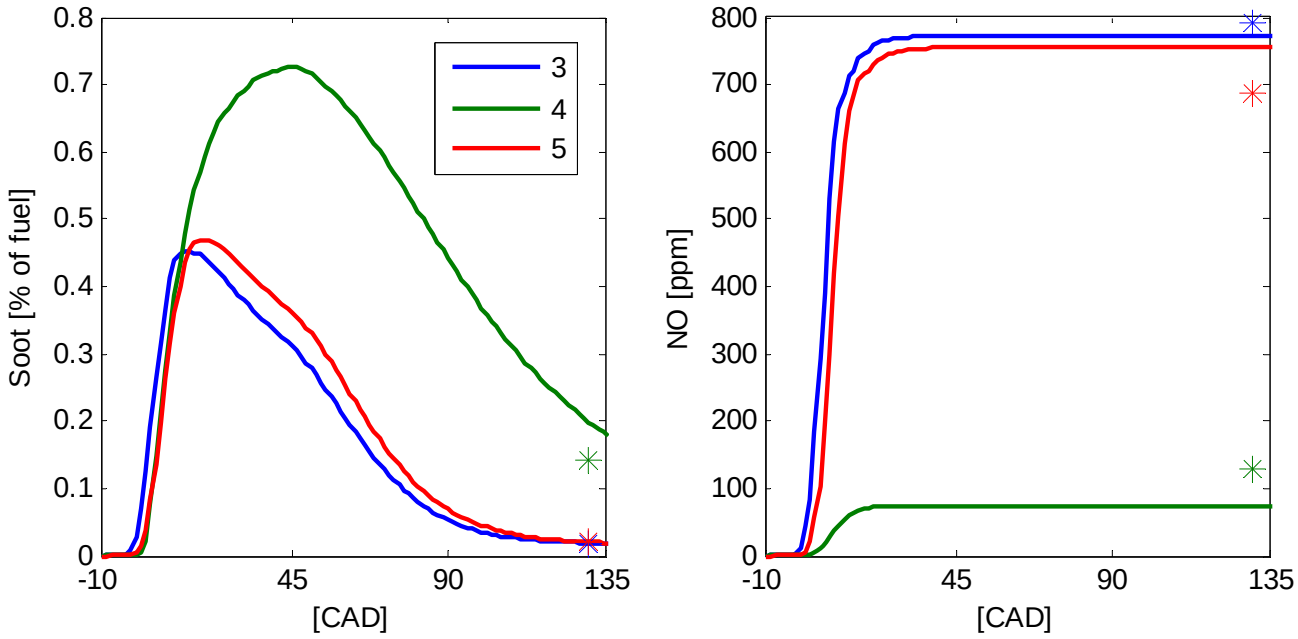

Figure 17 Crank angle resolved emission predictions. Case 3 and 5 are identical besides regarding injection angle. Case 4 and 5 are identical besides regarding EGR rate. The stars (*) show the measured values for the different cases.

7.4 Paper 4, "Fast Physical Emission Predictions for Off-line Calibration of Transient Control Strategies"

In paper 4, the models developed in paper 3 were used to predict the emission during transient operation. Similarly to paper 2, a full engine load transient was evaluated with different control strategies but this time with more strategies and also including soot. In this experiment, only measurements were used as inputs. Without making any changes to the models from paper 3, the predicted emissions agreed well with measurements, as shown in figure 18. In most cases where there are discrepancies in one of the predicted emissions, there is a corresponding discrepancy in the other and this probably means that these shortcomings origin from input data or modeling the in-cylinder conditions.

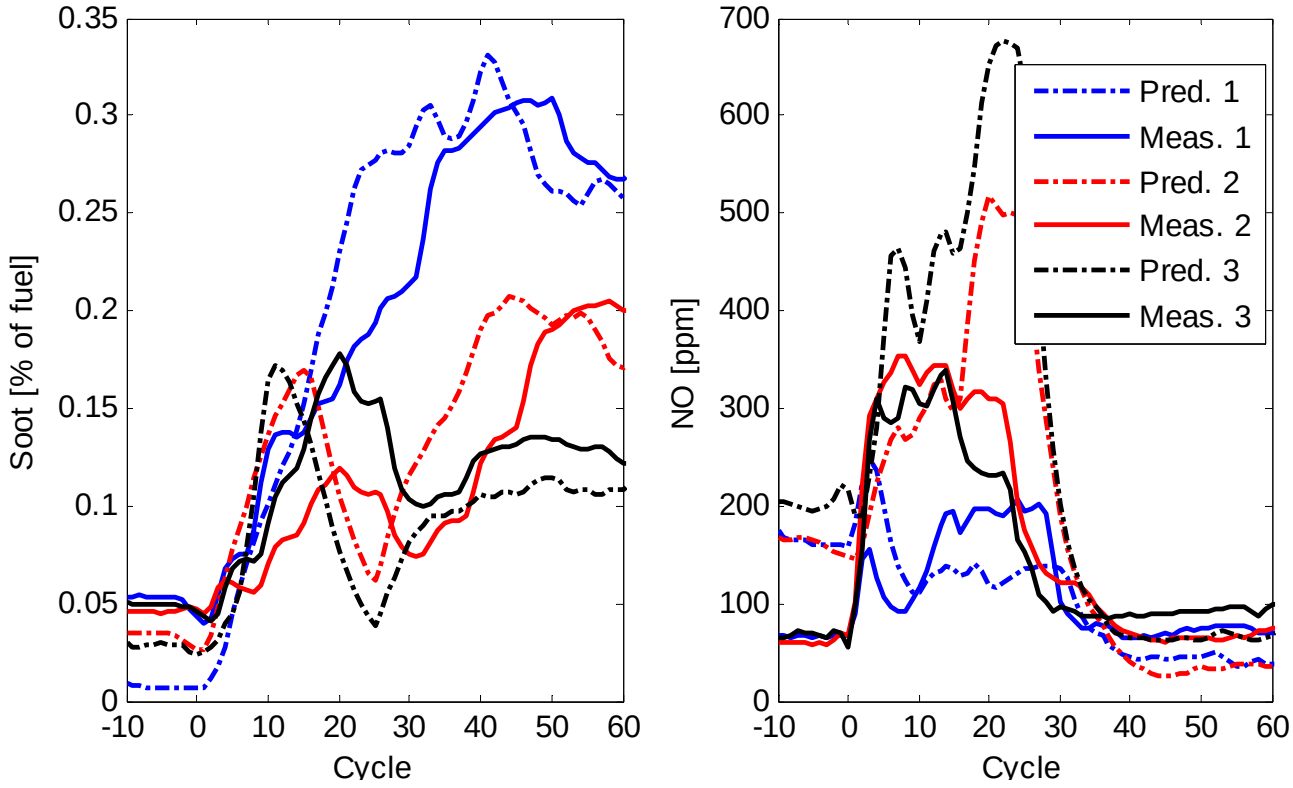

Figure 18 Predicted emissions during a load transient with three different strategies. The strategies are identical in case 1 and 2 besides the EGR-valve position during the first 10 cycles. Case 2 and 3 are identical besides the VGT position during the first 20 cycles of the transient

8 Summary

The long term objective for this project is to develop models that allow optimization of engine control strategies for transient operation via simulations. The motivation for this is the need for improved understanding of this operating condition and also a wish to minimize the time needed for calibration in an engine test bed.

The steppingstones towards that goal are identifying measurement methods that can resolve the transient behavior of the engine in terms of gas exchange flows and temperatures and in terms of emissions. Also to develop models that can predict that behavior. Due to the high number of possible control settings, an additional requirement for the models is low computational time.

At this point, halfway into the project, a range of measurement methods and simulation tools have been tested. Methods for measuring emissions with acceptable time resolution have been identified as well as acceptable methods to estimate the air/fuel ratio and EGR rate during transients. However, there is still room for improvements. No effort has yet been made to improve temperature measurements and this makes it impossible to resolve the dramatic variations in intake temperature that occur as the EGR valve is closed and opened during the transient.

Regarding the modeling objectives, models for soot and NOx emissions have been validated with a wide range of stationary operating conditions and for transient conditions and the models appear to be applicable for their purpose. However, simulated inputs have only been used in lesser extent when a 1-D model was used to predict an engines transient behavior and provide inputs to a multizone NOx model and more work is needed before the long terms objectives can be regarded as fulfilled.

9 Future work

Examples of areas where additional work is needed and/or would be interesting:

- To prove the validity of the emission modeling approach, it is necessary to verify it on other engines
- To test the models in their intended application, i.e. to use them with engine models, 1-D and/or mean-value models, to optimize transient control strategies.
- Since the models predict the in-cylinder emissions during the engine cycle, it would be interesting to compare the models with in-cylinder measurements
- One of the fundamental assumptions in the soot model is that a typical soot formation rate can be found for a specific engine. However, if an engine with variable injection pressure was used, the typical soot formation rate would most likely be different at different pressures and thereby also interesting to try to model.
- The largest sources of error for the transient emissions predictions are believed to be measured inputs such as EGR rate, air/fuel ratio and temperatures. It would be interesting to see how the emission predictions improved if these were improved.
- Investigate how the models can be adjusted or extended to improve the accuracy for predicting emissions in premixed combustion.
- Try more time steps/number of zones in the multizone to see how it affects the time requirement for the model and its accuracy.

10 Acknowledgements

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