Investigation and Modeling of the Regeneration of a Coated DPF

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MEK - FM - EP - 2011-07
July 2011
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MEK-FM-EP-2011-07

Master's Thesis, July 2011
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Release date: July 29, 2011
Category: 1 (public)
Edition: First
Comments: This report is part of the requirements to achieve the Master of Science in Engineering (MSc) at the Technical University of Denmark. This report represents 30 ECTS points.
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Preface

This thesis is submitted for the degree of MSc in Engineering Design and Applied Mechanics in the department of fluid mechanics, at the Technical University of Denmark, under the supervision of Jesper Schramm and Rasmus Cordtz.

The thesis presents the outcome of 5 months research on catalytical supported diesel particulate filter technology, by the means of regeneration with catalytic substrate applied on the filter in form of a coating and applied on an upstream diesel oxidation catalyst. The research is an extension of a collaboration project between A.P. Møller-Mærsk A/S, Haldor Topsøe A/S and DTU in the field of catalytically supported soot oxidation of a wall flow DPF, and the research will presumably continue further after the closure of this work.

The intention with this thesis has been to investigate different possibilities of removing the main part of the particulate matter from the exhaust from onboard diesel generators on large vessels. Experimental data from previous work on a GENSET L16/24 engine was supposed to be used for investigating optimal size of a retrofitted particulate filter for the engine. However, several interesting aspects regarding the particulate filter technology were discovered during the experiments, and elaborating these observations is important for the understanding of the technology. Thus there was no time left for running simulation models with the physical properties of the GENSET engine, however, several interesting observations and simulations regarding particulate filter regeneration are illustrated and discussed, and I do not feel that this presents a shortcoming of the project. To elaborate on the results to ensure a deep and correct understanding of the observations made is important for the further research.

I would like to use this opportunity to thank Anders Ivarsson and my supervisors Jesper Schramm and Rasmus Cordtz for their suggestions and useful
comments regarding the interpretation of the experimental results. I specially thank Rasmus for his involvement in the experimental work. Because of his thorough explanation of the experimental test setup, which he developed in 2010, and his help with the execution of the experiments I had results ready for analysis at an early stage of the project period. I would also like to thank Rasmus for his engaging and constructive talks. These conversations have presented me with a broader understanding of the study and his engagement to the project has been encouraging throughout the period.
Abstract

Forthcoming legislation to near-land emissions from generator sets on ocean-going vessels will increase the requirements of aftertreatment technology on onboard diesel generators. The intention with this thesis is to investigate different possibilities of removing the main part of the particulate matter from the exhaust, with focus on the effect of catalytic coatings applied in diesel particulate filter (DPF) systems. Catalytic coatings can be placed on a catalyst substrate, i.e. a diesel oxidation catalyst (DOC), upstream the DPF or it can be applied directly on the DPF (CDPF). Alternatively in combined system including an un-coated filter (NC DPF) with an upstream DOC (CRT) or a DOC and a CDPF (CCRT).

Experiments based on raw exhaust gas sampling was conducted for the CDPF and the DOC for the purpose of investigating the performances regarding soot oxidation and conversion rates, and for calibrating a CDPF and a DOC model using the experimental data obtained. The CDPF results showed, what appeared to be, an improved soot burn rate in comparison to experimental results from previous in-house NC DPF tests, however, when presenting the results with respect to the DPF soot mass the CDPF and NC DPF results were more resembling. Hence the magnitude of a possibly improved soot oxidation due to the catalytical coating on the CDPF could not be determined solely from the experimental results. Oxidation reactions of CO, HC and NO on the other hand were proved catalyzed both by the coating on the CDPF and the DOC.

The DPF soot mass was seen to have a large influence on the soot burn rate from a simulation with the calibrated CDPF model, and this strengthened the belief that the improved soot burn rate measured for the CDPF with respect to the NC DPF should be considered with caution. In general the simulations gave no further impression that the CDPF coating enhances the soot oxidation noticeably, regardless of the catalyzed NO₂ production. The upstream NO₂ production catalyzed by the DOC on the other hand
showed effective influence on the soot oxidation in the DPF when simulating a CCRT and a CRT system. Moreover the DOC experiments showed a noticeable oxidation of solid soot in the DOC, as a reduction in the exhaust gas soot concentration of approximately 50% was seen over the DOC at approximately 500°C.

From the DPF regeneration perspective it was demonstrated with the DPF model that it is possible to maintain continuous regeneration with adequately \( NO_2 \) concentrations and temperatures. Dimensioning a DPF for a larger engine is easier if continuous regeneration can be considered, since the average soot mass then can be determined, and moreover will be rather constant. The possibility of triggering an \( O_2 \) based regeneration by idle gas conditions was also presented. This method can rapidly clean the DPF if a certain amount of soot is stored in the DPF (>8kg_{soot}/m^3_{DPF}), and exhaust and DPF monolith temperatures are adequate (550°C) when the idle conditions are initiated.
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Nomenclature

Abbreviations

\begin{itemize}
\item \textit{BPT} \ Balance Point Temperature
\item \textit{CCRT} \ Aftertreatment system with a DOC installed upstream a CDPF
\item \textit{CDPF} \ Coated Diesel Particulate Filter
\item \textit{CRT} \ Aftertreatment system with a DOC installed upstream a NC DPF
\item \textit{DOC} \ Diesel Oxidation Catalyst
\item \textit{DPM} \ Diesel Particulate Matter
\item \textit{NCDPF} \ Non-Coated Diesel Particulate Filter
\item \textit{RES} \ Raw Exhaust Sampling System
\item \textit{TC} \ Thermocouples
\end{itemize}

Symbols

\begin{itemize}
\item \textit{A}_{\text{front}} \ Frontal surface of the filter \quad m^2
\item \textit{bmep} \ Break Mean Effective Pressure \quad \text{Pa}
\item \textit{BP} \ Break Power \quad kW
\item \textit{c}_{k}^L \ Concentrations of species k in the reactive surface layer \quad kmol/m^3
\item \textit{CO} \ Dry Exhaust Gas Concentration of \textit{CO} \quad ppm
\item \textit{CO}_2 \ Dry Exhaust Gas Concentration of \textit{CO}_2 \quad \%
\item \textit{d}_{TC} \ TC diameter \quad mm
\end{itemize}
\[ E_a \quad \text{Activation energy} \quad \text{kJ/kmol} \]
\[ F \quad \text{Engine Force} \quad \text{kp} \]
\[ f_{sc} \quad \text{Soot permability} \quad \text{m}^2 \]
\[ f_{sd} \quad \text{Depth filtration permability} \quad \text{m}^2 \]
\[ f_w \quad \text{Wall permability} \quad \text{m}^2 \]
\[ G_{\text{air}} \quad \text{Air flow rate} \quad \text{kg/h} \]
\[ G_{\text{exh}} \quad \text{Exhaust mass flow rate} \quad \text{kg/h} \]
\[ G_{\text{fuel}} \quad \text{Fuel Flow rate (fuel consumption)} \quad \text{kg/h} \]
\[ h \quad \text{Heat transfer coefficient} \quad \text{W/m}^2\text{K} \]
\[ H_a \quad \text{Absolute humidity of intake air} \quad \text{g_{water}/kg_{dry\text{air}}} \]
\[ HC \quad \text{Dry Exhaust Gas Concentration of HC} \quad \text{ppm} \]
\[ HCR \quad \text{Hydrogen to carbon ratio of fuel} \quad 23/12 \]
\[ H_d \quad \text{Absolute humidity of dilution air} \quad \text{g_{water}/kg_{dry\text{air}}} \]
\[ H_u \quad \text{Lower Heating Value of Fuel} \quad \text{kJ/kg} \]
\[ K \quad \text{Reaction pre-factor} \quad 1/K_s\text{or 1/s} \]
\[ k \quad \text{Thermal conductivity} \quad \text{W/mK} \]
\[ k_A \quad \text{Arrhenius frequency factor} \quad \text{variable} \]
\[ k_w \quad \text{CDPF Thermal conductivity} \quad \text{W/m} \cdot \text{K} \]
\[ l_{plug} \quad \text{Length of CDPF inlet/outlet plugs} \quad \text{m} \]
\[ M \quad \text{Molar mass of dry air, (28.97)} \quad \text{g/mole} \]
\[ m_f \quad \text{Mass of collected particles/soot in sample filter} \quad \text{mg} \]
\[ m_{\text{fuel}} \quad \text{Fuel Flow Rate} \quad \text{kg/s} \]
\[ MG \quad \text{Molar Mass} \quad \text{kg/kmol} \]
\[ M_{\text{PT}} \quad \text{Particulate Mass Flow Rate} \quad \text{g/h} \]
\[ M_{\text{sam}} \quad \text{Mass of diluted exhaust passed through the sample filter} \quad \text{kg} \]
\[ m_{sc} \quad \text{Volume specific soot loading in the cake layer} \quad \text{kg/m}^3 \]
\[ m_{sd} \quad \text{Volume specific soot loading in the depthlayer} \quad \text{kg/m}^3 \]
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Unit</th>
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<tr>
<td>N</td>
<td>Engine speed</td>
<td>rpm</td>
</tr>
<tr>
<td>$p_a$</td>
<td>Saturation vapor pressure of intake air</td>
<td>kPa</td>
</tr>
<tr>
<td>$P_{amb}$</td>
<td>Ambient Pressure</td>
<td>Pa</td>
</tr>
<tr>
<td>$p_d$</td>
<td>Saturation vapor pressure of dilution air</td>
<td>kPa</td>
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<tr>
<td>PM</td>
<td>Particulate mass</td>
<td>g</td>
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<tr>
<td>$P_{S,1}$</td>
<td>Wet perimeter of the free inlet channel</td>
<td>m</td>
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<tr>
<td>PT</td>
<td>Soot mass rate</td>
<td>g/h</td>
</tr>
<tr>
<td>q</td>
<td>Dilution ratio</td>
<td>–</td>
</tr>
<tr>
<td>$q_w$</td>
<td>CDPF Specific heat</td>
<td>J/kg · K</td>
</tr>
<tr>
<td>R</td>
<td>Universal Gas Constant, (8.314472)</td>
<td>J/Kmole</td>
</tr>
<tr>
<td>r</td>
<td>General reaction rate</td>
<td>kmol/m³/s</td>
</tr>
<tr>
<td>$R_a$</td>
<td>Relative humidity in ambient air</td>
<td>%</td>
</tr>
<tr>
<td>$R_d$</td>
<td>Relative humidity of dilution air</td>
<td>%</td>
</tr>
<tr>
<td>$R_{sc}$</td>
<td>Soot regeneration rate in the cake layer</td>
<td>kg/m³/s</td>
</tr>
<tr>
<td>$R_{sd}$</td>
<td>Soot regeneration rate in the depth layer</td>
<td>kg/m³/s</td>
</tr>
<tr>
<td>spfc</td>
<td>Engine specific fuel consumption</td>
<td>g/kWh</td>
</tr>
<tr>
<td>$T_A$</td>
<td>Arrhenius activation temperature</td>
<td>K</td>
</tr>
<tr>
<td>$T_{amb}$</td>
<td>Ambient temperature</td>
<td>°C</td>
</tr>
<tr>
<td>$T_d$</td>
<td>Temperature of dilution air</td>
<td>°C</td>
</tr>
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<tr>
<td>$T_{wall}$</td>
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<td>$V_d$</td>
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<td>$V_s$</td>
<td>Volume Flow through flow meter/sample filter</td>
<td>m³</td>
</tr>
<tr>
<td>$y_g$</td>
<td>Mole fraction</td>
<td>mol/mol</td>
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<tr>
<td>$y_k^L$</td>
<td>Molefraction of species k in the reactive surface layer</td>
<td>kmol/kmol</td>
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**Dimensionless Numbers**

| AFr   | Air/fuel ration | –    |
$Nu$ Nusselt number

$Re$ Reynold’s number

$S_{sc}$ Switch for soot cake layer deposition

$S_{sd}$ Switch for soot depth layer deposition

**Greek Letters**

$\delta_d$ Sublayer thickness $mm$

$\epsilon$ Emissivity

$\eta_t$ Total Efficiency

$\lambda$ Air Fuel ratio

$\rho_{sc}$ Soot packing density $kg/m^3$

$\rho_{sd}$ Depth filtration threshold $kg/m^3$

$\rho_w$ CDPF Density $kg/m^3$

$\sigma$ Stephan Boltzman constant (5.670e-8) $W/m^2K^{-4}$

$\zeta$ CDPF loss coefficient

Chapter 1

Introduction

1.1 Background

As pollution from cars, trucks, and land-based stationary sources has been more tightly controlled over the last 40 years, the contribution of ships and port operations to air pollution in port cities has become more important. Thus more stringent requirements to near-land emissions from generator sets on ocean-going vessels are issued by several regulatory parties including IMO/MARPOL and EPA. According to EPA [4] the final MARPOL Annex VI 2014 standards will require high efficiency catalytic emission controls capable of reducing particulate matter emissions by 90% and NOx emissions by 80%, along with large reductions of hydrocarbon, carbon monoxide, and air toxic emissions [25].

Meeting these new standards will increase the requirements of aftertreatment technology on onboard diesel generators, and the intention with this thesis is to investigate different possibilities of removing the main part of the particulate matter from the exhaust. In this context Diesel Particulate Filter (DPF) systems will be investigated, with focus on the effect of catalytic coatings. Catalytic coatings can be placed on a catalyst substrate, i.e. a diesel oxidation catalyst (DOC), upstream the DPF or it can be applied directly on the DPF (CDPF). Alternatively in combined system including an un-coated filter (NC DPF) with an upstream DOC (CRT) or a DOC and a CDPF (CCRT).

In the recent years Haldor Topsoe AS (HTAS) has been a major contributor in the field of catalytically supported soot oxidation of a wall flow DPF.
in collaboration with the Mechanical Department at the Danish Technical University (DTU-MEK). At the DTU test facility a large number of DPF tests has been conducted, and research in this area has been ongoing at DTU-MEK the last years as a collaboration project between A.P. Møller-Mærsk A/S, Haldor Topsoe A/S and DTU. An auxiliary engine of the type GENSET L16/24 was donated from MAN B&W Diesel A/S to Københavns Maskinmesterskole (KME) in 1999 and was installed for testing of a DPF for onboard generators at DTU in 2004, and the project was carried out in the period 2006-2009.

Such tests requires expensive test equipment and are rather time consuming since a broad range of different DPF conditions must be investigated. To avoid the expensive and time consuming tests it was proposed to develop simulation models for investigating the best possible aftertreatment solutions for retrofitting in an auxiliary engine.

1.2 Objective

In this work the aim is to develop a DPF simulation model fitted to predict the behavior regarding soot oxidation of a HTAS coated DPF. Another purpose of this model, which not will be included in this work, is to determine the optimum size of a retrofitted DPF in an auxiliary engine. Further the purpose is to develop a DOC simulation model for analyzing the benefits of installing a DOC upstream the DPF. Before the simulation models can be calibrated further experimental data needs to be obtained. For convenience the necessary tests are conducted with a 1.4 liter DLD-414 Ford/PSA engine, as it can easier be used at stable conditions and is moreover less expensive to run than the GENSET engine.

To distinguish between catalytic and thermal soot oxidation in the DPF HTAS provided two Silicon Carbide filters. The two DPFs are of the wall flow type, and one is with a catalytic coating (CDPF), and the other is without (NC DPF). At DTU spring 2010 several tests were run on the latter type, by Cordtz [11] as a part of his work, where a very accurate sampling method for measuring the DPF soot burn rate was developed. In this work the same test setup will be used for individual tests on both the CDPF and a DOC with various inlet gas conditions. The experimental results from the NC DPF tests will be used for comparison to the CDPF tests, to achieve further knowledge of the effects of the catalytic coating on the CDPF.

The commercial software package AVL BOOST v2010 based on 1D modeling will be used for the simulations. BOOST offers a number of predefined regeneration models. However the model needs to be calibrated against experiments. In the work of (Cordtz, 2010) a model was calibrated for the
1.3 Outline

NC DPF, which provides a theoretical foundation for the simulations that will be performed in this work.

1.3 Outline

A short review of diesel engine emissions and aftertreatment technologies are given in chapter 2. The aftertreatment technologies reviewed are limited to the DOC and the wall flow DPF, including the catalytical coating. In chapter 3 the experimental procedure is reviewed. The raw exhaust sampling system is illustrated and described, and the individual test procedures for the DPF and the DOC are explained. Technical data of the test equipment is also found in this chapter.

The experimental test results are presented in chapter 4. The performance of the CDPF is measured by the soot burn rate as the parameter for describing the regeneration ability, and the effect of the catalytic coating on the CDPF is analyzed by comparing the results to the NC DPF (Cordtz, 2010/2011) [11, 12]. The pressure drop over the CDPF and the BPT is also presented, together with a discussion of why BPT not should be used as a universal measurement, and the insecurities regarding BPT as a measurement for comparing the two DPFs performances. The test results in terms of gas concentrations, considering exhaust emissions and conversions, are presented for both the DOC and the CDPF, and the soot oxidation in the DOC is evaluated.

Chapter 5 presents the simulation models with implementation and analysis. The DPF model is explained in terms of soot deposition and regeneration, and model initiation parameters and boundary conditions are given for both the DPF and the DOC model. The regeneration reactions, which follows an Arrhenius type expression, are calibrated in terms of activation energies and pre-factors, and the DPF catalytic wall reactions and the DOC oxidation reactions in terms of frequency factors and activation temperatures. The simulations regarding the single CDPF will comprehend an investigation of the influence of the soot mass in the CDPF with regards to the soot burn rate, an investigation of regeneration optimization and an evaluation of the model temperature dependency.

An empirical expression for the soot burn rate will be suggested and implemented in the DOC model such that CCRT and CRT systems can be modeled with respect to the overall system soot burn. Moreover the regeneration and the species conversions of the CDPF, CCRT and the CRT are compared.

Conclusions and suggestions are given in chapter 6, and discussions are included in the two chapters containing experimental or simulated results.
Chapter 2

Review of Diesel Engine emissions and after treatment technologies

2.1 Diesel Exhaust Emissions

The composition of diesel exhaust varies considerably depending on engine type, operation conditions, fuel lubrication oil and whether an emission control system is present. A large part of the exhaust gas is made up of air and some other harmless components, however diesel emissions consist of a wide range of noxious compounds, both regulated and non-regulated. Typical concentration of diesel exhaust gas components are shown in table 2.1.

The focus for reduction of harmful diesel emissions is mainly on particulate matter (PM) and NOx, [17]. Both components are harmful to health and are present in relatively large quantities. There are also strict legislations regarding HC and CO emissions, [2].

2.1.1 NO\textsubscript{x}, NO\textsubscript{2} and NO

NOx is formed as a result of the high combustion temperature and pressure in combination with a superstoichiometric amount of oxygen. Nitrogen dioxide NO\textsubscript{2} transforms in the air to form gaseous nitric acid and toxic organic nitrates, and nitric oxide NO can be oxidised in air to form nitrogen dioxide. Both NO and NO\textsubscript{2} participate in ozone layer depletion and have
CHAPTER 2. REVIEW OF DIESEL ENGINE EMISSIONS AND AFTER TREATMENT TECHNOLOGIES

<table>
<thead>
<tr>
<th>Component</th>
<th>Concentration</th>
<th>Unit</th>
</tr>
</thead>
<tbody>
<tr>
<td>$N_2$</td>
<td>70-75</td>
<td>vol %</td>
</tr>
<tr>
<td>$O_2$</td>
<td>5-15</td>
<td>vol %</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>2-12</td>
<td>vol %</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>2-10</td>
<td>vol %</td>
</tr>
<tr>
<td>$CO$</td>
<td>100-1000</td>
<td>ppm</td>
</tr>
<tr>
<td>$HC$</td>
<td>50-500</td>
<td>ppm</td>
</tr>
<tr>
<td>$NO_x$</td>
<td>30-600</td>
<td>ppm</td>
</tr>
<tr>
<td>$SO_x$</td>
<td>proportional to fuel S content</td>
<td>ppm</td>
</tr>
<tr>
<td>$PM$</td>
<td>20-200</td>
<td>mg/m$^3$</td>
</tr>
<tr>
<td>aldehydes</td>
<td>0</td>
<td>mg/mile</td>
</tr>
<tr>
<td>ammonia</td>
<td>2</td>
<td>mg/mile</td>
</tr>
<tr>
<td>cyanide</td>
<td>1</td>
<td>mg/mile</td>
</tr>
<tr>
<td>benzene</td>
<td>6</td>
<td>mg/mile</td>
</tr>
<tr>
<td>toluene</td>
<td>2</td>
<td>mg/mile</td>
</tr>
<tr>
<td>PAH</td>
<td>0.3</td>
<td>mg/mile</td>
</tr>
</tbody>
</table>

Table 2.1: Typical diesel exhaust gas components, Ref.[17]

Furthermore an indirect effect to global warming, [5]. The use of internal combustion engines has drastically increased the presence of nitric oxides in the environment.

2.1.1.1 NO$_2$ versus NO

In the atmosphere $NO$ and NO$_2$ concentrations will be in equilibrium depending on the daylight and ozone concentration, thus the groundlevel $NO/NO_2$ ratio is not important with respect to atmospheric chemistry, however, NO$_2$ is highly toxic for humans, hence a favorable $NO$ ratio is preferable considering health issues. When it comes to legislations there has previously not been separate restrictions regarding $NO$ and NO$_2$, only regarding the total amount of NO$_x$, hence the priority of the industry has been in terms of NO$_x$ emissions. However, as NO$_2$ is more toxic than NO a limit of 40µg/m$^3$ was required by the European Union from 2010 in city streets [2] and is today significantly surpassed in many cities [10].
2.1 Diesel Exhaust Emissions

2.1.2 Diesel Particulate Matter

Diesel particulate matter (DPM or PM) is mainly composed of elemental carbon (soot), ash and volatile compounds derived from unburned and partially burned fuel and lubricating oil and sulfate. Soot particles are formed by the incomplete combustion due to locally fuel rich regions in the combustion chamber, while the volatile compounds transform from gas phase to particle phase as the exhaust cools and dilutes with ambient air in the atmosphere.

In general diesel particulate is composed of agglomerates of small (10-30 nm) spherical particles and chain agglomerates in the size range of 40-500 nm in diameter. Other particles can be either a stand-alone metallic ash, derived from the lubricating oil, fuel containing additives, or metallic ash that has joined the soot particles. The composition of DPM varies greatly depending on the engine technology, test conditions, and in the case of sulfate particulates, the sulfur content in the fuel.

Soot is in the general category of airborne particulate matter, and is considered hazardous to the lungs and general health. There are specially concerns about ultrafine and nanoparticles as particles of this size means an increased number and surface area at same mass exposure. Also particles less than 5 $\mu m$ in diameter are not filtered out by the upper respiratory tract, and this yields all particles emitted from diesel engines. Another issue when it comes to PM is that atmospheric dilution and cooling of hot diesel exhaust may trigger the nucleation of new particles such as semi-volatile hydrocarbons and sulfuric acid. [19].

Emissions of NOx and particulate are coupled in the way that if oxygen partial pressure is reduced to reduce NOx emissions in the exhaust this will lead to more soot formation. On the other hand if better combustion is pursued to reduce the emissions of particulate this often leads to better oxidation conditions, and increased NOx emissions can be a result. Hence technologies to reduce PM emissions may or may not reduce NOx emissions. Technologies to reduce PM emissions can be in the form of advanced or alternative diesel fuels or advanced engine and pollution-control technologies.
2.2 Diesel exhaust gas aftertreatment technologies

For emission reduction the first option to be considered is the prevention of harmful emissions, however as emission regulations become more stringent, especially for NOx and PM, exhaust aftertreatment is becoming a primary method to produce certifiable engines. Several types of aftertreatment systems exists, included diesel particulate filters, diesel oxidation catalysts and lean NOx catalysts, and the former two will be discussed in the following section.

2.2.1 Diesel Oxidation Catalysts

A Diesel Oxidation Catalyst (DOC) converts a large part of the hydrocarbon compounds present in the soluble organic portion of PM emissions, as well as gaseous hydrocarbons, carbonmonoxide, aldehydes and mutagenic emissions.

In general catalytic converters consist of a monolith honeycomb substrate coated with platinum group metal catalyst, packaged in a stainless steel container. The honeycomb shaped configuration with many small parallel channels presents a high catalytic contact area to exhaust gasses, and the catalyst coating is designed to trigger the chemical reaction. Figure 2.1 shows a DOC from Dinex AS where the substrate structure is a metal support structure made from alternating layers of flat and corrugated metal foil.

![Figure 2.1: The Dinex DOC with metallic based substrate, Ref.[3]](image)

The diesel exhaust is typically lean, implying high levels of $O_2$ concentrations, and the DOC performs a range of oxidation functions by utilizing the oxygen available in diesel exhaust. NO, CO and hydrocarbon emissions are utilized through the following oxidation reactions:
In addition to this the catalyst exhibits a very high activity in the oxidation of the organic fraction (SOF) of diesel particulates to carbon dioxide and water, at low temperatures. However, at higher temperatures the oxidation catalysts release sulfates \( (SO_4) \) through the oxidation, meaning a counter-productive process which outweighs the benefit of the SOF reduction may occur in the catalyst. This does on the other hand strongly depend on the sulfur content of the fuel, thus it is not important today, after commercial introduction of low sulfur fuels.

In a study preformed by the Manufacturers of Emission Controls Association (MECA) a PM reduction of approximately 30 % was obtained using an oxidation catalyst and in combination with a fuel-borne catalyst a reduction of 42 % was obtained [6]. It was also reported that for optimum performance, a diesel catalyst at least equivalent to the engine displacement volume is desirable, meaning that for large diesel engines the catalyst optimal size is quite large for practical use.

In general catalysts have little effect at low exhaust temperatures, and only a limited effectiveness with particulates. Additionally they do not remarkably change the emissions of oxides of nitrogen, however, given the sizeable emission reduction in HC, CO and aldehydes, DOCs are good candidates for aftertreatment systems to be combined with another form of aftertreatment (i.e. diesel particulate filters) or with fuel-borne catalysts.

2.2.2 Diesel Particulate Filters

The diesel particulate filter (DPF) is the commonly used exhaust gas after-treatment device that reduce the tailpipe PM emissions by mass as well as by particle number, and is the most efficient after-treatment device. Several types of ceramic and sintered metal DPFs have been developed. The most successful and the most commonly used commercially, are porous ceramic wall-flow filters. Latest research have shown that DPF filtration efficiency can be as high as 99 %, in case of monolithic wall flow filters, [11, 13, 22].
CHAPTER 2. REVIEW OF DIESEL ENGINE EMISSIONS AND AFTER TREATMENT TECHNOLOGIES

In the DPF operation it is common to distinguish between filtration/loading and regeneration. The DPFs have a high soot load capacity, it is the regeneration which presents a challenge. Both the filter itself and the accumulated soot impose additional back-pressure to the engine, which is undesirable as it leads to an increased fuel consumption and a reduction in available torque. At high exhaust temperatures the accumulated particulate in the filter is oxidized by passive regeneration, however at lower temperatures active regeneration is necessary to burn off the soot. Particulate filter regeneration strategy can include catalysts, engine control and fuel injection. Whereas the most simple and effective are based on catalysts, either in form of fuel with catalytic additives or by catalytical coatings. Catalytic coatings can be placed on a catalyst substrate, i.e. a diesel oxidation catalyst (DOC), upstream the DPF or it can be applied directly on the DPF (CDPF). Alternatively in combined system including an un-coated filter (NC DPF) with an upstream DOC (CRT) or a DOC and a CDPF (CCRT).

2.2.2.1 Balance Point Temperature

The temperature at which soot accumulation is balanced by soot burn is called the Balance Point Temperature (BPT). The balance point temperature is a characteristic number used by many manufactures to describe the DPF performance. It is determined from the differential pressure curve. At moderate gas temperatures a partial soot oxidation takes place in the DPF, but still not enough to avoid soot accumulation in the filter, hence the pressure is continually increasing, however, at some point during further temperature increment the accumulation will stop and the pressure curve will stagnate. In this situation the soot burn rate is in equilibrium with the inlet soot flow rate, and the temperature at this state is called the BPT. At higher temperatures the pressure drop starts to decrease, and a regeneration of the DPF is initiated.

The Balance Point Temperature is highly dependent on engine, test procedure and exhaust composition. It is a function of operation conditions such as initial soot mass and inlet gas and soot composition, hence it can not be universally measured or evaluated from simulations, [24].

2.2.2.2 The monolithic wall flow filter

There are several geometric configurations for DPFs at the market; assembled parallel plate wall-flow elements, cylindrical cartridges, foam monolithic blocks and plates, concentric tubular wall-flow elements and wall-flow monoliths. Where the latter design remains the most popular. It has an extruded honeycomb structure, and is made from porous ceramic material. Several
filter materials are available, whereas two of them are commonly established: Cordierite and Silicon Carbide. Cordierite is a synthetic ceramic developed for flow through catalyst substrates and subsequently adapted for the filter application, and is the most popular filter media. Silicon Carbide (SiC) is the second most popular media, and has a higher melting temperature and better durability in high thermal stress applications than Cordierite. On the downside it has a higher weight and is more expensive.

The wall flow principle is illustrated in fig. 2.2. As seen the wall flow monolith has a channel structure, with every second channel plugged from alternate ends. This way the exhaust is forced through the porous substrate walls which provides the filtration as a mechanical filter, and the purpose of the catalytic coating is to lower the temperature needed for conversion of the soot that is in direct contact with the filter surface. The main advantage of the wall flow DPF is the high surface area per unit volume in addition to the high collection efficiencies.

The collection of soot and ash is sketched in Fig. 2.2. Ash, which may be present in aged filters, will form an ash plug at the end of the inlet channel, as well as a layer over the entire length of the filter. The presence of an ash layer will increase the overall pressure drop as there is additional flow resistance and a reduced free frontal surface in the inlet channel.

The collection mechanism can be categorized in two principal ways; deep-bed (depth) filtration and cake (surface) filtration.

In the depth filtration, the mean pore size of the filter media is larger than the mean diameter of collected particles, and the deposition occurs within the inertial structure of the medium. The particles are deposited on the media through a combination of depth filtration mechanisms such as; diffusional deposition, inertial deposition and flow stream interception.

Cake filtration is when the particulate is deposited on the channel wall through sieving. In cake filtration the particles are generally larger than
the sizes of the pores in the filter media, thus they form a deposition on
the medium known as filter cake. Cake filtration occur by a combination of
blocking, which is larger particles captured by sieving, and bridging, which
occurs when the particles smaller than the pore size in the filter medium
form a cake. The latter typically happens when the particle concentration
is large and two particles are about to enter a pore simultaneously.

The wall-flow monoliths work through a combination of depth and surface
filtration. The characteristic form of the law for constant pressure filtration
is

\[
\frac{d^2 t}{dV^2} = k_1 \left( \frac{dt}{dV} \right)^{k_2}
\]  

(2.4)

where \( k_1 \) and \( k_2 \) are constants. \( k_1 \) dependent on the initial flow rate, and
\( k_2 = 2, 1.5, 1 \) or 0 for complete blocking, standard blocking, intermediate
blocking and cake filtration respectively, [30].

2.2.2.3 Coated Diesel Particulate Filters

In the catalytically coated DPF the porous walls of the monolith are covered
with an active catalyst in which purpose is to assist soot burning by forming
more \( NO_2 \) for the oxidation reaction. In addition the catalytic coating
has the function of combusting hydrocarbons and carbon monoxide both
during passive and forced regeneration, [18]. For a CDPF, the regeneration
is expected to take place at lower temperatures than for the NC DPF, and
thereby increase the soot burn efficiency, because the regeneration activation
energy will, in theory, be reduced by the participation of the catalysts in the
reaction process.

The main conception of the catalytic coating on the CDPF is to oxidize
the \( NO \) so additional \( NO_2 \) is available for the soot oxidation. As \( NO_2 \) is
formed along the length of the filter, some \( NO_2 \) is only formed downstream
of some of the soot. However, \( NO \) that has been formed from the oxidation
of particulate can also be re-oxidized over the catalytical coating so even
more \( NO_2 \) is available for further soot oxidation. The contribution of \( NO_2 \)
is important in the regeneration, as it will react with the soot \( C(s) \) in the
DPF to form \( NO \) and \( CO \) or \( CO_2 \) the following way:

\[
C(s) + NO_2 \rightarrow CO + NO
\]  

(2.5)

\[
C(s) + 2NO_2 \rightarrow CO_2 + 2NO
\]  

(2.6)
A restriction with the catalyzed filters is that only the particles in direct contact with the catalytic coating are able to oxidize, and the reduction in soot ignition temperature is rather small (30-100°C), thus a thermal regeneration back-up device, for forced regeneration, is still needed, [21]. Another drawback is the generation of sulfates by catalytic oxidation of the exhaust $SO_2$ to $SO_3$. The gaseous $SO_3$ can penetrate the porous walls and combining with water it forms sulfate particulates that increase the total output of particulate matter, [17]. However, this is only relevant in case of fuels with high sulfur content.

### 2.2.2.4 Catalytic systems, CRT and CCRT

The CRT (Continuously Regenerating Technology) system is the most widely used DPF system in the world and is a patented Johnson Matthey technology. The CRT system is composed by a DOC followed by an uncoated DPF, for interest see [7, 16]. The oxidation catalyst removes $CO$ and $HC$ and oxidizes some of the $NO$ in the exhaust gasses to $NO_2$, as described in sec. 2.2.1. This $NO_2$ then can react with the soot in the filter, producing $NO$ and $CO_2$ and cleaning the filter. In case of a CDPF some of the produced $NO$ is then re-oxidized to $NO_2$ in the filter, which then reacts with more of the trapped particulate. The DOC in combination with a coated DPF (CDPF) is called CCRT (Catalyzed Continuously Regenerating Technology). The major advantage of the CCRT over the CRT is the wider range of operating conditions, see table 2.2. The advantage of the CCRT and CRT compared to the single CDPF is that the $NO_2$ is formed upstream of the DPF, and therefore has a higher possibility of getting in contact with the soot layer on top of the filter walls. The patents expired in the US in April 2008 and in Europe in April 2009, thus anyone can offer these configurations to the market today.

Koltsakis et. al investigated the performance of catalyzed particulate filters without upstream oxidation catalyst, [14]. The effectiveness of a single CDPF towards reducing the gaseous $CO$ and $HC$ emissions was investigated and the behavior of single CDPFs was compared with DPFs comprising an

<table>
<thead>
<tr>
<th></th>
<th>Operating conditions</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>min. temp. for 40% of the operating time</td>
<td>NOx/PM ratio</td>
</tr>
<tr>
<td>CRT®</td>
<td>260°C</td>
<td>25</td>
</tr>
<tr>
<td>CCRT®</td>
<td>210°C</td>
<td>15</td>
</tr>
</tbody>
</table>

**Table 2.2:** Operating conditions for the CRT and CCRT system

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upstream DOC. They claim that the single CDPF is a viable and cost-effective option with a comparable efficiency and max temperature to the CRT/CCRT system if the filter soot loading is controlled at levels below a carefully selected threshold. Moreover it has been concluded from several research projects that the performances of the three systems discussed can be ranked as follows: CCRT > CRT > CDPF, [24, 27].
In this chapter the test procedure for the experiments will be described together with an illustration of the sampling system, which is based on Raw Exhaust gas Sampling. The technical data for the test engine, the particulate filter and the catalyst used are listed in this chapter, and there is a short review of the parameter sensitivity in the experiments.

3.1 Experimental methods and procedures

The substantial of the test setup is that the DPF/DOC is exposed to real engine exhaust, and the PM flow entering the DPF/DOC is measured to correctly determine the soot regeneration rate. The method is furthermore easy to operate and condensation effects caused by exhaust gas and dilution air mixing are avoided due to the raw gas sampling. The sampling system based on Raw Exhaust gas Sampling (RES), was developed at DTU spring 2010 by Cordtz as a part of his study ref.[11]. This set up has been proven to be a very accurate sampling method, hence no modifications or preliminary testing is necessary.

3.1.1 Raw Exhaust Sampling System

A sketch of the test facility setup is shown in fig.3.1. Basically the RES system contain four main components; sample filter, cooler, vacuum pump
The heart of the RES system is the sample filter, which is a downscaled SiC DPF of the wall flow module (size 1/68 of DPF). During a test sample gas is continuously extracted from the main exhaust gas and directed through the sample filter. The flow through the filter is typically around 4.5 kg/h and is maintained by the vacuum pump, which in turn is connected to a flow meter. The filter housing is equipped with nozzle heaters used to maintain the temperature at 180°C to reduce effects of thermo-diffusion of soot on walls. However, the temperature should not exceed 250°C to ensure that no soot oxidation can happen.

The sample filter provides a high filtration capacity. The module is embedded in a sealed filter housing of stainless steel, with a Pall Flex Emfab membrane filter located downstream to filtrate the finest particles. It is connected to a sample probe in the exhaust pipe, located either before the DPF/DOC or after the DOC. To meet close to isokinetic sampling conditions at all exhaust flow rates the optimum probe diameter was found by Cordtz, 2010 to be 30 mm. The tube connecting the sample probe and the filter is as short as possible to minimize any losses, and to minimize soot depositions on tube wall both tube and probe are constructed in stainless steel.

The cooler is a pneumatic air cooler with a flow capacity of 600 l/min and is used to remove water and thereby spare vacuum pump and flow meter. The water is collected and the measured mass is added to the mass of the sample gas passed through the flowmeter.
The CDPF or DOC is installed in an extended exhaust pipe from the engine, which is insulated all the way upstream the installation. It is installed between flange modules as seen in fig. 3.2.

3.1.2 RES test procedure and data post-processing

Before each test calibration of gas analyzers and heating of sample equipment is assured. Each test is performed at steady state conditions, meaning the engine speed and load are fixed. The desired engine load is controlled by an Eddy Current Brake which allow operations with steady state power and acceleration rate.

During experiments the DPF/DOC inlet and outlet centerline gas temperatures and pressure drop are measured using transducers and thermocouples (TCs), and the analog output signals are transmitted to a computer using LabVIEW. From a preliminary temperature field investigation of the NC DPF (Cortz, 2010) [11] it was found that the filter temperature remained almost unchanged over the cross section and length of the NC DPF (max variation from inlet-center to outlet-circumference was found to be 9%), and concluded that to simplify the test procedure a mean temperature of the centerline inlet and outlet was sufficient to define an overall temperature.

Emissions of $CO_2$, $CO$, $HC$, $NO_2$ and $NO$ upstream and downstream the DPF/DOC are measured using various gas analyzers, and the concentrations are logged by the computer. A three way valve allows to change between measuring at inlet and outlet. From the exhaust pipe the exhaust sample gas passes a heated (180 °C) PTFE sample hose before entering the analysers. The analysers measures dry concentrations, which can be converted to wet based concentrations using the meteorological conditions of pressure, temperature and relative humidity.

The concentration of soot (PM) is determined from the collected filtrated particles in the sample filter, which is found from the mass difference of filter before and after a test, measured using a digital scale. In short the particu-
late mass flow rate at the DPF/DOC inlet is calculated by the sampled soot concentration from:

\[
PT_{in} = \frac{M_f}{M_{sam}} \cdot (G_{exh} - G_{sam}) \quad [g/h] \quad (3.1)
\]

Where \( G_{sam} \) and \( G_{exh} \) is mass flow rate of sample and exhaust gas respectively. \( M_f \) is the filtrated soot mass in the sample filter, and \( M_{sam} \) is the exhaust mass past through the sample filter and flow meter calculated using the ideal gas law based on properties of dry air. There is a small leak in the vacuum pump which causes false air to enter the system, meaning the flow through the flow meter is somewhat diluted. This is accounted for in the calculations, and the computational methods used can be seen in Appendix B.1.2. All calculations and illustrations are made using Matlab®.

### 3.1.3 CDPF test procedure

During each test the CDPF is running in the cake regime, which is when the pores of the SiC material is filled with soot. In-house experience with the filter arrangement has shown that the SiC material itself can filtrate more than 99% of the soot mass when the filter is working in the cake filtration regime, therefore only the exhaust soot concentration upstream the CDPF is sampled to provide the supplied soot flow rate of the CDPF and the very low soot concentration downstream is neglected.

Ahead of the tests conditioning is preformed, as was discovered to be necessary in the work by (Cordtz, 2010) [11]. The background and procedure of the conditioning test is further described in the proceeding section, 3.1.4. After each test, including the conditioning, both filters are disassembled and weighed. The sampling filter is weighed immediately after the engine is turned off, while the CDPF is weighed when the temperature has dropped to 140°C.

In 2010 Cordtz [11] found that the soot mass could be predicted precisely by weighing the filters in ambient conditions, as long as the filters had the same individual temperature before and after the test, hence the filter temperatures are assured to be consistent in advance of all measurements.

The tests duration time is slightly more than two hours. Within the first minutes the CDPF and sampling filter is subjected to idle gas conditions, then the engine load is applied, and the first pairs of emission measurements are taken when the exhaust temperature and gas conditions have reached a steady state, typically after approximately 20 min.
The average DPF soot burn rate of a test is in short found as the difference between the particulate mass flow rate at the CDPF inlet, from eq. (3.1), and the stored soot mass inside the CDPF, calculated as the filtrated soot mass in the CDPF during the test length $M_{sam}/t_{test}$ in [g/h].

$$PT_{DPF,burned} = PT_{DPF,in} - PT_{DPF,stored} \ [g/h] \ (3.2)$$

### 3.1.4 CDPF conditioning and $O_2$ storage

It was discovered by (Cordtz, 2010), ref.[11] that the RES system needed to be preheated and conditioned before real DPF test could be preformed. The preheating of the engine and exhaust system is typically around 25 min, and once the engine is stopped the sample filter is disassembled, and the sample filter weight is recorded immediately after. During system conditioning soot will deposit/diffuse onto the internal walls of the probe, sample tube and the filter housing. At some point this effect is neutralized and accurate soot samples can be preformed.

The necessity of preheating and conditioning is rather intuitive. There was, however, discovered another phenomena by Cordtz, namely DPF $O_2$ storage. The coating on the HTAS CDPF contains the rare earth metal cerium, which is able to store and release oxygen. Due to the high amount of $O_2$ stored in the CDPF, (2.5 g/h), the soot mass samples did, in 2010, not match the actual soot mass ($PT_{filtrated} \neq PT_{sampled}$). Thus, conditioning was discovered to be a necessity in order to fill the DPF with oxygen in advance of the tests.

In (Cordtz, 2010) [11] one hour preconditioning with $T_{exh} \approx 230^\circ C$ was

![Figure 3.3: Measured temperature during CDPF conditioning](image3.3)

![Figure 3.4: Measured differential pressure during CDPF conditioning](image3.4)
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attempted, however, this was inadequate for the CDPF. Therefore the pre-
conditioning was preformed with a higher exhaust temperature in this ex-
periment ($T_{exh} \approx 350^\circ C$). The measured temperature and pressure is seen
in fig. 3.3 and 3.4 respectively.

For the NC DPF no soot burn was detected at 304$^\circ C$, thus the first CDPF
test is run with corresponding temperature. The sampled soot mass was
calculated to be 3.36 g/h, and the measured soot mass was slightly less, 3.0
g/h. Hence the understanding is that the chosen conditioning procedure was
sufficient to complete the $O_2$ filling of the CDPF.

3.1.5 DOC test procedure

Since the DOC does not collect any particles the test procedure is slightly
different from the setup for the DPF test. For the DPF tests it is adequate to
sample exhaust soot concentration upstream the DPF, however when testing
the DOC it is necessary to sample both at the DOC inlet and outlet. Since we
only possess one sampling filter the sampling has to be done in two rounds,
thus it is very important to have the same steady state condition during the
whole test, to ensure same flow condition and hence same particulate flow
rate at the DOC inlet.

Each test length last slightly more than two hours, with approximately one
hour of sampling upstream the DOC followed by one hour of sampling down-
stream the DOC. Before the tests starts the desired engine load is applied,
and during heating of the engine there is no exhaust gas passing through
the sampling filter. When steady state temperature and gas concentrations
are reached the valve at the sample filter inlet is opened and the vacuum
pump started. After one hour the sample filter is disassembled and weighed
and moved from the DOC inlet to the DOC outlet.

The average DOC soot burn rate of a test is found as the difference in
the particulate mass flow rate sampled before and after the DOC, both
calculated from eq. (3.1).

$$PT_{DOC,burned} = PT_{DOC,in} - PT_{DOC,out} \quad [g/h] \quad (3.3)$$

3.1.6 Temperature corrections

The exhaust gas temperature upstream and downstream the CDPF/DOC
is measured by thermocouples (TCs). In most cases the raw measurements
are used directly, however, the signal from a TC can deviate from the actual
temperatures due to factors such as thermal capacitance of the tip itself,
and heat transfer to the exhaust pipe wall through conduction and radi-
3.1 Experimental methods and procedures

ation. Thus, to enhance the accuracy of the exhaust gas inlet and outlet temperatures, all measurements have been corrected by setting up an energy balance of the TC wire installed in the exhaust system. The computational method for this correction is found from ref. [29], and is shown in appendix B.1.4, where it is shown that the TC cooling is caused mainly by radiation heat transfer between the TC and the surrounding pipe wall. Therefore a better location for the TC could be inside a DPF channel where heat radiation to pipe walls can be neglected, however that would mean blocking a filter channel, and thereby miss the soot accumulation in that channel.

3.1.7 Parameter sensitivity

In the work done by (Cordtz, 2010) ref.[11] a sensitivity analysis of the experimental data used as inlet boundary conditions for the simulations in BOOST was made. It was then concluded that the accuracy of meteorological parameters play a very small role in the calculation of soot burn rates. The most important parameters were found to be $CO_2$ concentrations, sampled soot mass $m_f$, sample flow $V_{sam}$ and fuel consumption $G_{fuel}$.

To ensure accurate measurements of these parameters the following is done:

- $CO_2$: All sample line leakages are removed and pretest calibration of gas analyzers are confirmed before each test
- $V_{sam}$: Validated against another flowmeter
- $G_{fuel}$: Three measurements are performed and averaged for each test
- $m_f$: Filters are measured at same temperature after each test and are treated carefully
3.2 Technical data of test equipment

In this section the technical data for the DPFs, the HTAS DPF coating, the DOC, the test engine, the test fuel and silicon carbide is listed.

3.2.1 HTAS-Coated DiSiC DPF

Haldor Topsøe A/S (HTAS) provided two Silicon carbide filters for testing purposes at DTU. The two DPFs are of the wall flow type, and one is with a catalytic coating (CDPF), and the other is without (NC DPF).

The DiSiC® filter is fabricated by the danish company Dinex AS. The SiC filter technology used in the DiSiC system is designed as a honeycomb structure with every second channel blocked, forcing the exhaust gasses through the micro porous wall, separating the particulate from the gas [3].

The monolith is processed in segments divided by cement stripes to compensate for the high thermal expansion coefficient of the filter material (SiC). The inlet and outlet channels are square in shape but with different hydraulic diameters, asymmetrical channel diameters. This structure improves the filtration capacity. The physical parameters for the DiSiC DPF are listed in table 3.1. The wall thickness between the inlet and outlet channel can be calculated from the following formula, ref. [9]

\[
\delta_{wall} = \sqrt{\frac{4}{\text{cpsi}\cdot1550}} - d_1 - d_2
\]  

(3.4)

<table>
<thead>
<tr>
<th>DPF type</th>
<th>Wall flow</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monolith material</td>
<td>SiC</td>
</tr>
<tr>
<td>Coating material</td>
<td>Palladium, Pd</td>
</tr>
<tr>
<td>Monolith diameter/length</td>
<td>140/252 mm</td>
</tr>
<tr>
<td>Monolith volume</td>
<td>3.88 l</td>
</tr>
<tr>
<td>Channel density [cells per square inch]</td>
<td>196 cpsi</td>
</tr>
<tr>
<td>Inlet/outlet channel hydr. diameter</td>
<td>1.7/1.3 mm (asymmetric)</td>
</tr>
<tr>
<td>Wall thickness between inlet and outlet</td>
<td>0.21 [mm]</td>
</tr>
<tr>
<td>Total weight (clean CDPF)</td>
<td>5022.7 g</td>
</tr>
</tbody>
</table>

(Calculated from (3.4) ref.[9])

Table 3.1: DPF specifications
3.2 Technical data of test equipment

3.2.1.1 Novel base metal-palladium CDPF coating

The CDPF coating is a novel base metal-palladium catalytic diesel filter coating developed by HTAS. The catalytic coating is termed BMC-211, and the Pd content is 1.5 g Pd/l.

Most commonly used are platinum based coatings, however, the metal-palladium coating coating has shown comparable soot combustion, $HC$ conversion and $CO$ conversion properties, and does additionally possess $NO_2$ reducing properties, ref. [18]. The BMC-211 coating produces $NO_2$ to be utilized for soot oxidation at high temperatures, while for temperatures below 330° C the $NO_2$ amount is significantly reduced. This makes this coating especially usable in connection with a normal Pt-DOC in front of the filter. Moreover the HTAS CDPF contains cerium.

3.2.1.2 Silicon carbide

Silicon carbide (SiC) is a chemical material which is widely used as filtration material for DPFs. The combination of an excellent soot collection rate and low backpressure performance qualifies SiC to be a superior material for filtering soot particles. As mentioned, in-house experience with the filter arrangement has shown that the SiC material itself can filtrate more than 99% of the soot mass when the filter is working in the cake filtration regime. The specifications of SiC in the DiSiC filter can be seen in table 3.2.

<table>
<thead>
<tr>
<th>SiC parameters</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Coefficient of Thermal Expansion [(CTE)/°C]</td>
<td>$40 - 45 \times 10^{-7}$</td>
</tr>
<tr>
<td>Melting temperature [°C]</td>
<td>2400</td>
</tr>
<tr>
<td>Intrinsic Density [g/cm$^3$]</td>
<td>3.24</td>
</tr>
<tr>
<td>Spe. Heat Capacity @ 500°C</td>
<td>0.95</td>
</tr>
<tr>
<td>Axial E-Modulus [GPa]</td>
<td>33.34</td>
</tr>
<tr>
<td>Porosity</td>
<td>$40 - 60%$</td>
</tr>
<tr>
<td>Pore diameter</td>
<td>$10 - 20\mu m$</td>
</tr>
<tr>
<td>Catalytic coating (compared to Cordierite)</td>
<td>$More suitable$</td>
</tr>
<tr>
<td>Cost (compared to Cordierite)</td>
<td>$High$</td>
</tr>
<tr>
<td>Use (compared to Cordierite)</td>
<td>$Segmented$</td>
</tr>
<tr>
<td>Thermal shock resistance (compared to Cordierite)</td>
<td>$Less$</td>
</tr>
<tr>
<td>Mechanical strength compared to Cordierite</td>
<td>$Less$</td>
</tr>
</tbody>
</table>

Table 3.2: SiC specifications
3.2.2 Dinex Diesel Oxidation Catalyst

A DOC from Dinex AS is used for the experiments. The substrate structure in the DOC is a metal support structure made from alternating layers of flat and corrugated metal foil. The Dinex DOCs contain a loading of platinum ranging from 5 to 50 grams of platinum per cubic feet, depending on raw emission, application, fuel quality, and temperature. The catalyst material used is precious metal included in a wash coat, coated on a ceramic or metallic substrate.

<table>
<thead>
<tr>
<th>DOC type</th>
<th>Dinex (Metallic based substrate)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Platinum loading</td>
<td>5-50 g</td>
</tr>
<tr>
<td>CH and CO conversion</td>
<td>80-95%</td>
</tr>
<tr>
<td>Lifetime</td>
<td>3-6 years</td>
</tr>
<tr>
<td><strong>DOC size</strong></td>
<td></td>
</tr>
<tr>
<td>Diameter</td>
<td>132.5 mm</td>
</tr>
<tr>
<td>Length</td>
<td>118.5 mm</td>
</tr>
<tr>
<td>Monolith volume</td>
<td>0.001634 m$^3$</td>
</tr>
</tbody>
</table>

Table 3.3: DOC specifications

The Dinex DOCs are claimed to have 80-95 % conversion of $HC$ and $CO$ into $CO_2$ and water, and conversion of PM is said to only be related to the SOF and PM mass, without affecting the particle number. The DOCs are moreover expected to have a life time of 3-6 years and are maintenance free during that period, according to ref.[3].

3.2.3 PSA Diesel Engine

The test engine is a turbocharged 1.4 liter diesel engine taken from a Citroen C2, with specifications as seen in table 3.4. The engine is fabricated by Ford/PSA and the model number is DLD-414. The engine is equipped with a turbocharger and a high pressure common rail direct injection, and serves as a benchmark for a modern diesel engine for experimental work. The engine is also equipped with an EGR (Exhaust Gas Recirculation) valve which reduces the NOx emissions from the engine, however this is turned off during the tests. The engine power is absorbed by an Eddy Current Brake, where the break power ($BP$) is given in kilo pounds ($kp$). The calculation methods used to calculate the engine performance parameters can be seen in Appendix B.1.1.
3.2 Technical data of test equipment

<table>
<thead>
<tr>
<th>Engine type</th>
<th>PSA 1.4 HDI</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of cylinders</td>
<td>4</td>
</tr>
<tr>
<td>Compression ratio</td>
<td>17.9:1</td>
</tr>
<tr>
<td>Displacement volume</td>
<td>1398 cm$^3$</td>
</tr>
<tr>
<td>Power</td>
<td>50 kW @ 4000 rpm</td>
</tr>
<tr>
<td>Torque</td>
<td>150 Mm @ 4000 rpm</td>
</tr>
</tbody>
</table>

Table 3.4: Test engine specifications

3.2.3.1 Test fuel specifications

The fuel used in the experiments is a common low sulphur fuel as described in table 3.5.

<table>
<thead>
<tr>
<th>Fuel type</th>
<th>Shell Diesel Extra 10</th>
</tr>
</thead>
<tbody>
<tr>
<td>Lower heating value</td>
<td>42.7 MJ/kg</td>
</tr>
<tr>
<td>Sulphur content</td>
<td>&lt; 10 ppm</td>
</tr>
</tbody>
</table>

Table 3.5: Test fuel specifications
Experimental results and discussion

In this chapter the test results from the CDPF and the DOC tests will be presented and discussed in terms of temperatures, including the balance point temperature, pressures, soot burn rates and gas concentrations, considering exhaust emissions and conversions. The effect of the wash coat on the CDPF is analyzed by comparing the results to the NC DPF (Cordtz, 2010/2011) [11, 12]. Last the boundary conditions necessary to generate the simulation model in BOOST are summarized.

4.1 CDPF test results

Five steady state tests, with exhaust temperature range from $\sim 300 - 450^\circ$C, was conducted with the CDPF for the purpose of investigating the effect of the catalytical coating with respect to oxidation of soot (PM), hydrocarbons, carbon monoxide and nitric oxides, and for calibrating a BOOST regeneration model for the CDPF. For comparison test results of the NC DPF will be presented. The measured exhaust properties and species concentrations are listed in appendix A.1. NC DPF properties are seen in A.1.3.

4.1.1 Measured temperatures and differential pressures

The measured centerline CDPF inlet and outlet temperatures are shown in figure 4.1. In each test a steady state condition was reached after ap-
Approximately 20 min, where the temperature stabilizes with a weak positive gradient.

Figure 4.2 shows the results from the NC DPF test, ref.[12], for comparison, and the measurements from the two experiments compare quite well at equivalent engine loads. In the NC DPF test the filter inlet and outlet temperature was almost identical, while there is a temperature drop over the CDPF, as seen in fig. 4.1.

Further the CDPF temperature will be based on a mean temperature adjusted with the corrections described in section 3.1.6 and appendix B.1.4. The temperature corrections are applied to compensate for factors such as thermal capacitance and heat transfer that can influence the signals from the TCs. The corrections are important, but not severely large, less than 5%, and can be seen in table 4.1.

Figure 4.3 and 4.4 illustrates the pressure drop over the CDPF and the NC

<table>
<thead>
<tr>
<th></th>
<th></th>
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<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>640</td>
<td>2500</td>
<td>37</td>
<td>317</td>
<td>326</td>
<td>273</td>
<td>282</td>
<td>305</td>
</tr>
<tr>
<td>2</td>
<td>768</td>
<td>2500</td>
<td>45</td>
<td>362</td>
<td>373</td>
<td>322</td>
<td>332</td>
<td>353</td>
</tr>
<tr>
<td>3</td>
<td>896</td>
<td>2500</td>
<td>52</td>
<td>400</td>
<td>413</td>
<td>340</td>
<td>352</td>
<td>383</td>
</tr>
<tr>
<td>4</td>
<td>1024</td>
<td>2500</td>
<td>60</td>
<td>427</td>
<td>443</td>
<td>363</td>
<td>377</td>
<td>411</td>
</tr>
<tr>
<td>5</td>
<td>960</td>
<td>3000</td>
<td>67</td>
<td>457</td>
<td>476</td>
<td>394</td>
<td>411</td>
<td>444</td>
</tr>
</tbody>
</table>

Table 4.1: CDPF Temperatures, temperature corrections and mean temperature
4.1 CDPF test results

DPF respectively. It can be noticed that the pressure drop relative to engine load is higher for the CDPF than for the NC DPF. The coating can cause a higher pressure drop, however there was overall more soot stored in the CDPF at the initiation of the tests than in the NC DPF, as seen in table 4.2, and this will participate to higher pressure drop over the CDPF.

<table>
<thead>
<tr>
<th>Power [%]</th>
<th>37</th>
<th>45</th>
<th>52</th>
<th>60 (61)</th>
<th>67 (68)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$m_{soot,init}$ [kg/m³]</td>
<td>1.50</td>
<td>1.69</td>
<td>1.45</td>
<td>3.01</td>
<td>4.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>NC DPF</th>
<th>CDPF</th>
</tr>
</thead>
</table>

Table 4.2: CDPF and NC DPF initial soot mass

The DPF balance point can be roughly estimated from figure 4.3 and 4.4 from the increasing or decreasing pressure drop tendency. For the CDPF the constant pressure curve is located somewhere between 52 and 60% engine load, thus $BPT < 411^\circ C$. For the uncoated DPF the balance point was not reached before between 68 and 73% load, indicating a BPT above $435^\circ C$, which seems to demonstrate a lower BPT for the CDPF.

In test 4, $T_{CDPF} = 411^\circ C$, the pressure is decreasing, thus the BPT was assumed to be located below this temperature, however, this is not necessarily the case. It is common to define BPT as when $\Delta p = 0$, however it is more correctly defined by the temperature where the soot loading and soot oxidation of the DPF is in equilibrium, and this was not the case for this test. The soot mass in the filter was in fact increasing during the test time, and despite this the pressure drop was decreasing. The importance of this observation will be further discussed in section 4.3.1.

Figure 4.3: Measured CDPF differential pressure

Figure 4.4: Measured NC DPF differential pressure, Ref.[12]
4.1.2 Measured soot concentration and soot burn rates

The RES sampling method provides an accurate mean value of the soot concentration, which is an important input parameter for the simulation model described later in this report. The soot concentration measured by the RES system is illustrated relative to exhaust temperature and engine power for both the NC DPF and CDPF in fig. 4.5. The presented concentrations are considered average soot concentrations $PM_c$ at the DPF inlet. The PM concentration is between 18 and 33 mg per kg exhaust for the CDPF, and is in general increasing with engine load. It can be noticed that regardless the similarity in engine power and exhaust temperatures there is a difference in PM concentration between the NC DPF and the CDPF experiments. This demonstrates the large difficulties when it comes to predicting how much soot an engine will release. The exhaust soot concentration does moreover influence the BPT, and for the BPT to provide a credible comparison of DPF efficiencies it is important to account for the inlet soot concentration.

Supplied, stored and average soot burn rates are presented in fig. 4.6. The soot burn rate displays an exponentially development with temperature, as also was discovered for the NC DPF, fig. 4.7. In test 5, $T_{CDPF} = 444^\circ C$, the stored soot rate is negative, indicating DPF regeneration. When the stored soot rate is zero the DPF soot burn rate equals the supplied soot rate, hence the BPT can be read as where the stored soot rate becomes negative. Thus $BPT_{CDPF} \approx 420^\circ C$ and $BPT_{NC\,DPF} \approx 460^\circ C$. However, the BPT depends on engine soot production and DPF soot mass, and neither of these parameters were equal for the two DPF tests, which means that the BPT

![Figure 4.5: Measured soot concentrations at DPF inlet from the CDPF and the NC DPF tests](image)
is not a reliable parameter for comparing the two filters. The temperature where soot oxidation is initiated and the oxidation rate at this temperature is possibly more important parameters to consider. There is no noticeable soot oxidation in the CDPF at 300°C, seen from the small difference between the supplied and stored soot rates in fig. 4.6. Thus it does not immediately seem like the activation temperature is reduced considerably by the catalytical coating on the DPF.

Figure 4.8 presents the average soot burn rates in comparison to the NC DPF. From the illustrated soot burn rates it appears as if the CDPF has an enhanced soot oxidation in comparison to the NC DPF.

Figure 4.6: Supplied, stored and average soot burn rates from CDPF tests

Figure 4.7: Supplied, stored and average soot burn rates from NC DPF tests, Ref.[12]

Figure 4.8: Average soot burn rates for the CDPF and th NC DPF
If the soot oxidation is occurring throughout the soot-cake layer, the overall soot mass in the filter, including the initial soot mass, will have an impact on the soot oxidation. In figure 4.9 the soot burn rate is presented as percent soot burn relative to the average soot mass in the filter, considering a test length of one hour after steady state conditions are achieved, calculations are seen in appendix B.1.3. The soot burn rates in the CDPF still show an improvement compared to the NC DPF, however, the difference is not as large as it appeared from the comparison of soot burn rates in fig. 4.8. This could be interpreted as if the increased soot burn rate for the CDPF compared to the NC DPF detected in figure 4.6 is more influenced by the DPF soot mass rather than the effect of the catalytic coating on the CDPF. This will be discussed further in section 5.1.

![Graph showing percent soot burn relative to average DPF soot mass for CDPF and NC DPF.](image)

**Figure 4.9:** Percent soot burn relative to average DPF soot mass for CDPF and NC DPF

### 4.1.3 Measured \( \text{NO}_2 \), \( \text{CO} \) and \( \text{HC} \) conversion

\( \text{NO}_2 \) can be utilized as a low-temperature soot oxidation agent, [27, 22, 32], and it is therefore interesting to see the \( \text{NO}_2 \) conversion rate over the CDPF. In figure 4.10 percent conversion of \( \text{NO}_2 \), \( \text{CO} \) and \( \text{HC} \) are illustrated for the CDPF compared to the NC DPF, increment in concentrations are presented as negative values. It can be understood from figure 4.10 (a) that \( \text{NO}_2 \) is formed in the CDPF due to the catalytic coating, since there is a negative conversion of \( \text{NO}_2 \) only for the CDPF. This occurs at temperatures above 380°C, showing an \( \text{NO}_2 \) production up to nearly 30% at 444°C. The \( \text{NO}_2 \) production might in reality be higher provided that some of the \( \text{NO}_2 \) is utilized for soot oxidation. The NC DPF shows a rather constant \( \text{NO}_2 \) reduction of \( \sim \)10%, and this reduction is also seen for the CDPF below...
350°C, which could indicate that the catalytical supported NO$_2$ reaction is inactive below this temperature.

As described in section 2.2.2 one of the conceptions of the catalytic coating on the filter is to oxidize NO in the filter wall so additional NO$_2$ is available for further soot oxidation. However, if the NO$_2$ is formed downstream the soot it could have a minor effect on the oxidation of particulate, while the exit NO$_2$ concentration is high, which is undesirable since NO$_2$ is more hazardous than NO. The NO$_2$/NO-ratio is presented in figure 4.11, and whether the additional NO$_2$ is utilized in the CDPF will be further discussed in chapter 5.

The NO$_2$ conversion in test 3, $T_{CDPF} = 383°C$, is more or less equal for
the CDPF and the NC DPF, thus there is no noteworthy additional NO$_2$ present for the soot oxidation in the CDPF, nevertheless the average soot burn rate is higher for the CDPF than the NC DPF, fig. 4.8. In fig. 4.9, on the contrary, where the soot burn rate is presented relative to the average soot mass in the filter, the CDPF and NC DPF results are resembling, which supports that the soot oxidation depends on the soot mass, and that presenting the relative behavior might give more authentic results.

The overall NO$_x$ emission is necessarily not influenced by the catalytic reaction, it is solely the NO$_2$/NO ratio that is affected, and as seen in fig. 4.12, the NO$_x$ emissions are not higher for the filter with coating. This supports the reaction equations in section 2.2.2, where soot C(s) reacts with NO$_2$ to form an equivalent amount of NO and CO or CO$_2$.

![Figure 4.11: Measured CDPF and NC DPF NO$_2$/NO-ratio](image1)

![Figure 4.12: Measured NO$_x$ concentration at CDPF and NC DPF inlet and outlet](image2)
In addition to being harmful components there are legislations regarding emissions of carbon monoxide and hydrocarbons, thus it is interesting to see the conversion rates of $HC$ and $CO$. The results as regards $CO$ and $HC$-removal are presented in figure 4.10 (b) and (c) respectively. Nearly all the carbon monoxide and approximately half the hydrocarbons are converted in the CDPF, compared to an insignificant conversion in the NC DPF. This verifies that in order to remove hydrocarbons and carbon monoxide, the DPF must be provided with a catalytic coating. However, in the proceeding section it will be presented that an upstream DOC is able to remove at least equivalent amounts of $HC$ and $CO$, as well as producing a higher amount of $NO_2$ to be utilized for soot oxidation in the DPF.
4.2 DOC test results

Five tests, with exhaust temperature range from \( \sim 300 - 500 \)°C, was conducted with the DOC for the purpose of investigating the DOC performance, and for calibrating a BOOST simulation model for the DOC. The measured exhaust properties and species concentrations are listed in appendix A.1.2.

![Figure 4.13: Measured DOC inlet (black) and outlet (blue) temperatures](image1)

The measured centerline DOC inlet and outlet temperatures are presented in fig.4.13, and as seen a steady state condition was reached after approximately 20 min. The plotted exhaust temperatures are adjusted with the corrections for the TC’s described in appendix B.1.4, and for the proceeding sections a mean temperature will be considered. Table 4.3 shows the DOC inlet and outlet temperatures.

<table>
<thead>
<tr>
<th>Test nr</th>
<th>Load [kpa]</th>
<th>Load [rpm]</th>
<th>Load [%]</th>
<th>( T_{\text{in}} ) [°C]</th>
<th>( T_{\text{corr,in}} ) [°C]</th>
<th>( T_{\text{out}} ) [°C]</th>
<th>( T_{\text{corr,out}} ) [°C]</th>
<th>( T_{\text{DOC}} ) [°C]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>627</td>
<td>2500</td>
<td>37</td>
<td>317</td>
<td>327</td>
<td>289</td>
<td>299</td>
<td>313</td>
</tr>
<tr>
<td>2</td>
<td>761</td>
<td>2500</td>
<td>44</td>
<td>367</td>
<td>379</td>
<td>336</td>
<td>349</td>
<td>364</td>
</tr>
<tr>
<td>3</td>
<td>896</td>
<td>2500</td>
<td>52</td>
<td>399</td>
<td>414</td>
<td>367</td>
<td>383</td>
<td>398</td>
</tr>
<tr>
<td>4</td>
<td>960</td>
<td>3000</td>
<td>67</td>
<td>462</td>
<td>483</td>
<td>427</td>
<td>447</td>
<td>465</td>
</tr>
<tr>
<td>5</td>
<td>886</td>
<td>3500</td>
<td>72</td>
<td>494</td>
<td>515</td>
<td>457</td>
<td>478</td>
<td>496</td>
</tr>
</tbody>
</table>

![Figure 4.14: Measured NC DPF inlet and outlet temperatures, Ref.[12]](image2)

Table 4.3: DOC Temperatures, temperature corrections and mean temperature

The reason for the sudden jump after \( \sim 90 \) min in the temperature curve for test 2 (\( T_{\text{DOC}} = 364 \)°C, 44% engine load), is that the test was performed over two different days, the first day sampling before DOC and the second day after the DOC. The total length of the test was 160 min. In test 5
(\(T_{\text{DOC}} = 496^\circ \text{C}, 67\% \text{ engine load}\)) the LabVIEW file was interrupted, hence the first minutes of the test are missing from the plot, this does, however, not influence any forthcoming results.

The differential pressures over the DOC was measured to be between 3 and 7 mbar, which means that the pressure drop over the DOC is only about 7% of the pressure drop over the CDPF.

![Graph](image)

**Figure 4.15:** Measured soot concentrations at DOC, CDPF and NC DPF inlet and DOC outlet

Figure 4.15 illustrates the measured soot concentrations at the inlet of the NC DPF, the CDPF and both the inlet and the outlet of the DOC. The sampling was, with exception of the second test, performed before and after the DOC while the engine was running continuously at steady state, hence there is no reason to suspect different soot concentrations at the DOC inlet during a test. Thus it is very interesting to see that the soot concentration at the DOC outlet is overall lower than at the inlet, and especially at the highest temperatures. At 496°C the soot concentration at DOC outlet is less than half of the concentration entering the DOC, which demonstrates a significant oxidation of solid soot in the DOC.

The measured soot concentrations at the DOC inlet are in general lower than in the CDPF and NC DPF test series, and once again the irregularities in engine soot production are underlined, as the inlet soot concentration deviates to such a degree, even at equivalent engine conditions. In the search for patterns regarding the soot concentration released from the engine the only comprehensible conclusion was that predicting the soot mass in engine exhaust is extremely difficult.

July 2011

DTU - MEK
The rate of soot oxidation for the DOC is viewed in fig. 4.16 in comparison to the two DPFs. Since the soot is not trapped in the DOC as it is in the DPFs, the soot burn rates does not actually compare. Still an exponential soot burn tendency is visual at the higher temperatures for the DOC, and it is conclusive that there is an important amount of soot oxidation present in the DOC.

![Figure 4.16: Average soot burn rates of the DOC, CDPF and NC DPF](image)

### 4.2.1 Measured DOC species conversion

As well as the the purpose of the DOC is emission reduction of \( HC \) and \( CO \), oxidation of nitric oxide to nitrogen dioxide is also an important role of the DOC when installed upstream a DPF. The contribution of \( NO_2 \) is important in the regeneration, as it will react with the soot \( C(s) \) in the downstream DPF to form \( NO \) and \( CO \) or \( CO_2 \) as described in section 2.2. As seen in fig. 4.17 (a) the \( NO_2 \) conversion is high, up to 50% additional \( NO_2 \) can be provided to the DPF by the DOC in the temperature range \( 400-450^\circ \text{C} \). From the figure it is moreover seen that there is no production of \( NO_2 \) below \( 350^\circ \text{C} \), thus the DOC will have no influence on the regeneration in a downstream DPF at such low temperatures.

It was observed that there is soot oxidation present in the DOC, thus the actual \( NO_2 \) production might be slightly higher since some \( NO_2 \) could possibly have been utilized for the oxidation of soot.

Other primary functions of a DOC is to catalyze the oxidation of carbon monoxide and uncombusted fuel (\( HC \)) to \( CO_2 \) and water, and these con-
4.2 DOC test results

Conversion rates are presented in fig. 4.17 (b) and (c) respectively. The CO reduction is rather stable at a conversion rate of ~90-95% for the entire test temperature range, and the HC reduction is slightly lower, approximately 80-85%.

![Figure 4.17](image)

Figure 4.17: DOC conversions of: (a) NO$_2$ (b) CO and (c) HC
4.3 Conclusive summary and discussion

The results from the tests of a HTAS coated CDPF and a Dinex DOC have been presented and evaluated. The purpose has been to investigate the DOC and CDPF performance, especially considering the effect of the catalytic coating on the CDPF. Another object was to identify the boundary conditions necessary for calibrating a BOOST simulation model for both the DOC and the CDPF.

4.3.1 CDPF experimental results

At first glance the CDPF results showed an improved soot burn rate compared to the NC DPF results, although, when presenting the soot burn rates with respect to the average DPF soot mass the improvement was less outstanding. The balance point temperature is lower for the CDPF, however, since the initial soot mass is higher in the CDPF tests, there are large uncertainties whether the BPT is a good parameter for describing the regeneration abilities of the two DPFs. The difference in inlet soot concentration between the two tests is also contributing to an increased uncertainty regarding the measured BPT, hence it was concluded that BPT not can be considered a reliable parameter for comparing the two filters.

Since physical parameters, such as DPF soot mass and exhaust gas soot and species concentration, influences the regeneration significantly, further study is preferable before making a final conclusion regarding the effect of the catalytic coating with regards to soot oxidation. The CDPF regeneration will be further investigated with simulations in the following chapter.

The catalytic coating on the CDPF did catalyze the oxidation reactions of $CO$, $HC$ and $NO$. A significant reduction of carbon-monoxide and hydrocarbons was achieved with the CDPF, practically 100% $CO$ conversion and approximately 50% $HC$ conversion was measured. No noticeable conversion of $NO_2$ was seen below $\sim350^\circ C$, but the production was nearly 30% at the highest measured temperature, $T_{CDPF} = 444^\circ C$.

4.3.1.1 Experimentally measured CDPF temperature drop

There was noticed a temperature difference between CDPF inlet and outlet. The temperature is an particularly important parameter since the soot burn rate is exponentially temperature dependent, thus to reassure that the measurements were correct, an additional control of the thermocouples (TCs) was preformed. Consistency was seen for the measured temperatures with the two TCs, and it was verified that the temperature measurements both upstream and downstream the CDPF showed accurate results.
Reactions with carbon monoxide and hydrocarbons are normally exothermic, and can potentially increase the CDPF temperature, hence the temperature drop over the CDPF, which was not noticed for the NC DPF, was unexpected. The simplest explanation for the different temperature gradients is the possibility of the NC DPF being better isolated than the CDPF, although there is no reason for suspecting so, as the two DPF monoliths should be identical. Another possibility could be that the catalytic coating enhances an endothermic reaction, which would explain why the temperature drop is limited to the CDPF. However, demonstrating an endothermic behavior is particularly difficult since regeneration in principle is an exothermic phenomenon, as it involves burning of carbon. In an experiment where cerium was used as a fuel additive it was discovered an endothermic phenomena in the DPF during regeneration, (Kyriakis, 2003) [26]. This phenomena was experimentally investigated and were found to be related to the cerium content of the fuel and to the soot mass accumulated in the DPF.

### 4.3.1.2 Experimentally measured CDPF pressure drop

The CDPF pressure drop was noticeably larger for the CDPF than for the NC DPF. In ref.[24], the increase in differential pressure for a CDPF compared to an NC DPF is explained by the structural difference between the coating and the wall material. Because of the catalytic coating the pores are smaller in the CDPF, thus the deep-bed filtration will occur much faster, and once the pores become plugged, the cake filtration will take place. However during both experiments the DPF was working in the cake regime, assuming no further depth filtration took place during the tests.

In the work done by (Cordtz, 2010) it was found that the catalytical coating only caused an additional pressure drop of a few mbar, and not nearly as much as the difference presented in this report, where the measured DPF pressure drops were up to 30 mbar higher for the CDPF than for the NC DPF. From this comparison it appears that the greater part of the additional DPF pressure drop over the CDPF was caused by the soot in the filter rather than the coating or the monolith. The initial DPF soot mass, which was larger in the CDPF tests than in the NC DPF tests, would influence the DPF pressure drop significantly.

In CDPF test 4, $T_{CDPF} = 411^\circ$C, the CDPF pressure drop was decreasing, although the soot mass in the CDPF was increasing, which means that something besides the overall change in DPF soot mass caused the negative gradient. This is an important observation, since it indicates that something changes in the soot layer during the the CDPF regeneration. It would be interesting to investigate whether this phenomena is limited to the CDPF or if the NC DPF shows similar behavior. However, within the time-frames
of this work, further testing cannot be accomplished. Knowledge about how the soot oxidation is behaving in the different soot layers in the DPFs is very limited, and it is difficult to conclude with certainty in what way the soot layer is influenced by the soot oxidation in the CDPF. This will be discussed further in chapter 5.

4.3.1.3 Absences and opportunities for further work

According to research by HTAS and DTU, ref.[15], the CDPFs have shown only small advantages in supporting $O_2$ based soot regenerations and catalytic DPF coatings does not have major influence on the $O_2$-C(s)-reaction. This matches the results from this experiment, however, in [15] it was found that catalytic coatings resulted in a faster, more complete regeneration in the temperature range of 540-640°C, which is above the temperature range of this experiment. Without using active regeneration, additional insulation or an external heat source temperatures in that range can not be achieved with this test setup, and a larger improvement in CDPF efficiency above the tested temperatures can not be excluded.

As mentioned, the temperature is a particularly important parameter when simulating the soot burn rate since it is exponentially temperature dependent, and defining the accurate inlet temperatures in BOOST is essential for obtaining a good simulation model. Using a mean DPF temperature was the obvious choice since the temperature progression in the DPF has not been investigated. However, if there is an endothermic reaction in the DPF caused by the catalytic coating it is plausible that the gas temperature in the inlet channels are higher than in the outlet channels, since the gas will have to pass the coating on the DPF walls before the endothermic reaction occurs. If this is the case defining a mean temperature as the inlet BC temperature in the simulation model is not completely correct, since the gas which interacts with the accumulated soot could have a higher temperature. Due to these uncertainties a temperature investigation of the CDPF would be beneficial. An experiment with several TCs placed in the outlet and inlet channels at different radial and axial positions were discussed, however, within the timeframes of the project it could not be achieved. Moreover it was concluded that using a mean temperature for the CDPF is a reasonable assumption.
4.3 Conclusive summary and discussion

4.3.2 DOC experimental results

The DOC experiment showed promising results regarding the DOC performance, considering both species conversion and soot oxidation.

4.3.2.1 Experimentally measured DOC soot burn rate

The rate of soot oxidation for the DOC was moderate compared to the two DPFs, however, it is remarkably high, considering that the soot is not trapped in the DOC as it is in the DPFs. This means that only the soot provided to the DOC during a test (~2h) can be oxidized, while the DPFs have stored soot from several hours of soot loading, which then can be oxidized at high temperatures. The soot burn rate moreover showed an exponentially tendency at the higher temperatures, as seen for the DPFs.

The soot concentration at the DOC outlet was overall lower than at the DOC inlet, especially for the highest temperatures. At 496°C, which was the highest test temperature in the experiment, the soot concentration at the DOC outlet was less than half of the concentration entering the DOC.

One concern regarding the soot burn in the DOC is whether the actual number of soot particles are reduced or only the particles size. This is a concern only if the DOC is installed without a downstream DPF, because, the smaller the soot particles, the more harmful they are to humans, [20, 28]. Hence the soot mass reduction in the exhaust gas is indifferent without reducing the number of particles if the gas is directly released to the atmosphere.

Therefore further testing of DOCs with respect to particle sizes will be necessary before a DOC can be used unsupported by a DPF for the purpose of particulate removal. However, in combination with a DPF the DOC has the potential of improving the reduction in particulate emission noteworthy.

The soot concentration released from the engine has been shown to be quite unpredictable, and the characteristics, (size, shape, porosity, composition), of the individual soot particles are expected to vary. This might influence the soot oxidation in the DOC significantly, and the soot burn rates in a second experiment will not necessarily correspond to the soot burn rates calculated from this series of tests. Hence further testing of the DOC is also necessary from the aspect of determining an average soot oxidation, seen that the results from the different test series deviates.
In this chapter a BOOST Diesel Particulate Filter Model and a BOOST Catalyst Model will be calibrated individually for investigating the CDPF and the DOC performances. The two models will then be implemented in combination to simulate the common regeneration system where a DOC is located upstream either a CDPF (CCRT) or an NC DPF (CRT).

During Cordtz’s work in 2010 ref.[11] a temperature field investigation over the cross section and the length of the DPF was made, and it was then found that the temperature at steady state conditions was nearly uniform over the DPF cross section, still the soot regeneration is likely most aggressive in the DPF core, and not uniform throughout the DPF cross section, as assumed in the 1D model. However, 1D modeling was concluded to be sufficient for simulating loading and regeneration behavior for the NC DPF, and AVL BOOST v5.1 was chosen for the task.

BOOST is is an advanced and fully integrated ”Virtual Engine Simulation Tool” with advanced models for accurately predicting engine performance, acoustics and the effectiveness of exhaust gas after treatment devices, and in this work AVL BOOST v2010 will be used for all simulations.
5.1 CDPF model calibration

The BOOST DPF code applies a solver for wall-flow type DPFs with asymmetric channel geometries in the presence of inlet/outlet plugs and various kinds of soot and ash distributions, fig. 5.1. The model calculates the pressure drop and the velocities in the inlet and outlet channel of the DPF as well as the corresponding wall velocity profile.

The effective filtration flow is described by 1D steady-state balance equations of continuity and momentum for a representative pair of inlet and outlet channels. From a user defined channel geometry the velocities and the associated pressure drops of the inlet and outlet channels are calculated by the BOOST code.

The total wall pressure drop is the sum of individual pressure drops given by the wall, a soot depth filtration layer, an ash layer and a soot cake layer, evaluated as mean values over the effective filter length, and Darcy’s law is applied for the calculation of the individual velocities over the different layers.

The soot deposition and regeneration approach in BOOST will be described in the preceding section. For further description of the filter flow modeling concept please refer to [9], chapter 4.

5.1.1 DPF soot deposition and regeneration model

Figure 5.2 shows the different soot, ash and wall layers considered in the BOOST DPF code. Soot reactions only take place in the cake and depth layer. The ash layer is assumed to be inert with respect to chemical reactions.
and ash mass is typically neglected due to long term effects, while the soot cake, the soot depth layer and the wall itself are considered reactive layers where soot regeneration and catalytic reactions can take place.

The two following soot balance equations are applied to capture the transient changing soot mass in both the cake and depth layer separately. Each equation describes the change in stored soot mass from the difference between a soot burn source term $\dot{R}_{sd}$ and a supplied soot rate $\dot{m}_{soot,inl}$.

\[
\frac{dm_{sd}(z)}{dt} = \dot{R}_{sd} + \overline{w}(z) \cdot \dot{m}_{soot,inl} \cdot S_{sd}
\]

\[
\frac{dm_{sc}(z)}{dt} = \dot{R}_{sc} + \overline{w}(z) \cdot \dot{m}_{soot,inl} \cdot S_{sc}
\]

where $m_{sd}(z)$ and $m_{sc}(z)$ are the DPF volume specific soot mass in the cake and depth layer at each axial position of the filter, respectively. $\overline{w}(z)$ represents a dimensionless wall velocity at each axial position, which is used to distribute the incoming soot $\dot{m}_{soot,inl}$ along the inlet channel. The local velocity magnitude depends on the local soot height. $\dot{R}_{sd}$ and $\dot{R}_{sc}$ describe general soot reaction source terms in the different layers. $S_{sd}$ and $S_{sc}$ are binary switches to control the soot deposition in the depth layer and cake layer respectively.

Soot deposition in the depth layer is switched off as soon as the depth filtration capacity is reached, while soot deposition in the cake layer is switched on as soon as the depth filtration layer has reached its full capacity.

The regeneration reactions take place along the streamlines of gas flow passing through the soot layers. An 1D isothermal, steady-state, fixed-bed model is applied for small soot slices given by an axial discretization, under the as-
assumption that transports affects are negligible in directions other than given by the wall velocity (direction $x$ in Fig. 5.2).

The global continuity of the gas phase is used to compute the soot burn source terms

$$u_w \cdot \frac{d\rho_g}{dx} = \sum_j S \left[ MG_j \cdot \sum_i v_{i,j} \cdot \dot{r}_i(y_g, T_s) \right]$$

(5.3)

where $v_w$ is the local wall velocity at each axial position, $\rho_g$ is the gas density and $x$ represents the spatial coordinate over the height of the soot cake, soot depth layer and filter wall. $MG_j$ is the molar mass of the species $j$, and $S$ notes the total number of species. The stoichiometric coefficient of the species $j$ in the reaction $i$ is given by $v_{i,j}$ that multiplies the molar reaction rate $\dot{r}_i(y_g, T_s)$ of the $i$th reaction. The total number of reactions is represented by $R$.

The right hand side of eq. (5.3) directly equals to changes in solid soot mass, because only reactions where solid soot is involved contributes to the continuity source.

The species conservation equation over the height of the soot cake, soot depth layer and wall is

$$u_w \cdot \rho_g \frac{dw_{j,g}}{dx} = MG_j \cdot \sum_i v_{i,j} \cdot \dot{r}_i(y_g, T_s)$$

$$-w_{j,g} \cdot S \sum_j \left[ MG_j \cdot \sum_i v_{i,j} \cdot \dot{r}_i(y_g, T_s) \right]$$

(5.4)

where $w_{j,g}$ represents the gas mass fraction of species $j$.

The first term on the right side considers changes in the species composition due to all reactions involved. The second term on the right side (chain rule) is the spatial derivative of the gas density at constant species fractions.

Eq. (5.3) and (5.4) represent an initial value problem that can be integrated from the top of the soot cake down to the bottom of the filter wall.

Assuming that the species gas composition does not change significantly over the length of the inlet channel, the initial conditions at the topmost layer are given by

$$\rho_g = \rho_g(z) \quad @ \quad x = 0$$

(5.5)

$$w_{j,g} = w_{j,g,\text{init}} \quad @ \quad x = 0$$

(5.6)
5.1 CDPF model calibration

The solution of the fixed-bed model, eq. (5.3)-(5.6), delivers overall soot reaction terms for both the cake and the depth layer. The volume specific mass sources from eq.(5.1) and (5.2) are proportional to the density differences over the corresponding height (direction $x$ in fig. 5.2) given by

$$
\dot{R}_{sc} = u_w \cdot \frac{P_{S,1}}{A_{front}} \cdot \left( \rho_g \big|_{x=0} - \rho_g \big|_{x=x_{soot,cake}} \right) \tag{5.7}
$$

$$
\dot{R}_{sd} = u_w \cdot \frac{P_{S,1}}{A_{front}} \cdot \left( \rho_g \big|_{x=x_{ash,cake}} - \rho_g \big|_{x=x_{soot,depth}} \right) \tag{5.8}
$$

where $A_{front}$ is the frontal surface of the filter and $P_{S,1}$ is the wet perimeter of the free inlet channel.

By integrating the fixed-bed model over the entire height of all layers source terms for the continuity, species and energy balance equations can be derived. The energy balance is needed to calculate the temperature development during DPF regeneration.

5.1.1.1 DPF regeneration reactions

BOOST offers a set of predefined regeneration models with $O_2$ and $NO_2$ as the reactive species for the oxidation of soot/carbon $C(s)$. The regeneration models can be applied to the cake and depth filtration layer with their individual set of reaction parameters.

At first approximation the $O_2$ – $NO_2$ regeneration scheme, which contains the four first reactions in table 5.1 will be applied. Besides the $NO_2$ and $O_2$ regeneration BOOST offers the catalytically supported reversible oxidation of $NO$ to $NO_2$, reaction 5 in table 5.1, which may be relevant when simulating regeneration of a coated DPF. The rate of the individual regeneration reactions are following an Arrhenius type expression, which gives the exponential dependence of the temperature and the rate constant $\dot{r}$ as shown below:

$$
\dot{r}_i = K_i \cdot e^{-\frac{E_{a_i}}{RT}} \tag{5.9}
$$

The depth layer regeneration can be deactivated in BOOST, assuming regeneration only takes place in the cake layer. This is done primary to implement the regeneration kinetics from the work done by (Cordtz, 2010) [11], where the assumption was made due to limited information about the depth layer, and because during normal operation cake filtration is most likely present.
50  CHAPTER 5. SIMULATION MODELS AND ANALYSIS

Stoichiometry      Reaction rate

1  $C(s) + \frac{1}{2}O_2 \rightarrow CO$      $f_{co} \cdot K_1 \cdot e^{\frac{-E_{oa}}{RTs}} \cdot [O_2]$  
2  $C(s) + O_2 \rightarrow CO_2$      $(1 - f_{co}) \cdot K_1 \cdot e^{\frac{-E_{oa}}{RTs}} \cdot [O_2]$  
3  $C(s) + NO_2 \rightarrow CO + NO$      $K_3 \cdot e^{\frac{-E_{oa}}{RTs}} \cdot [NO_2]$  
4  $C(s) + 2NO_2 \rightarrow CO_2 + 2NO$      $K_4 \cdot e^{\frac{-E_{oa}}{RTs}} \cdot [NO_2]$  
5  $NO + \frac{1}{2}O_2 \leftrightarrow NO_2$      $K_5 \cdot e^{\frac{-E_{oa}}{RTs}} \cdot \left(c_{NO} \cdot c_{O_2} \cdot \frac{c_{NO_2}}{K_{eq}(Ts)}\right)$

\[ f_{co} = \frac{1}{1 + 0.02 \cdot [O_2]^{0.21} \cdot e^{3000}} \]

Table 5.1: BOOST DPF regeneration stoichiometry and reaction rates

\( K \) — Pre-factor - Total number of collisions between fuel and oxidizer per second, regardless if it is leading to a reaction or not
\( \dot{r} \) — Rate constant - Number of collisions that result in a reaction per second
\( e^{\frac{-E_{oa}}{RTs}} \) — The probability that each collision will result in a reaction
\( K_{eq} \) — Equilibrium constant

The DPF code as described is calculating the soot layer as homogenous, and does not include differences in soot porosity in the soot oxidation considerations. The effect of a different soot structure will thus be implemented in the pre-factors and activation energies, which means that it is not possible to simulate transient differences in soot permeabilities in BOOST.

5.1.2 DPF model initiation and boundary conditions

The boundary conditions applied for the model are equivalent to the experimental data sets, table A.1 and A.2. The inlet boundaries are exhaust temperature \( T_{exh} \), mass flux \( G_{exh} \), gas fraction and solid mass fraction. The only required outlet boundary is the exit pressure \( p_{DPF,out} \).

The DPF general properties and type specification can be seen in section 3.2.1. The physical properties of the DPF monolith are extracted from ref.[11] and are listed in table 5.2.

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5.1 CDPF model calibration

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Density</td>
<td>$\rho_w$ 3200 kg/m$^3$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>$k_w$ 38.5 W/m·K</td>
</tr>
<tr>
<td>Specific heat (@ T = 25°C)</td>
<td>$\varsigma_{lw}$ 750 J/kg·K</td>
</tr>
<tr>
<td>Specific heat (@ T = 800°C)</td>
<td>$\varsigma_{lw}$ 1250 J/kg·K</td>
</tr>
</tbody>
</table>

Table 5.2: DPF physical properties

The DPF model discretization is made as an 1D structure with 50 equally sized axial grid points, and the simulation is adiabatic, i.e. no heat loss to the surroundings.

The DPF has only been running few hours prior to the tests for this work, and there are no noticeable changes of the ash mass within the time ranges given by soot loading and regeneration events. Hence ash deposits, which may be present in aged filters, is neglected.

The soot and filter properties used initially was calibrated by (Cordtz, 2011) [12], and are listed in table 5.3. For the soot mass initiation the measured initial soot mass is inserted.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soot packing density</td>
<td>$\rho_{sc}$ 100 kg/m$^3$</td>
</tr>
<tr>
<td>Soot permability</td>
<td>$f_{sc}$ *1.9e-14 m$^2$</td>
</tr>
<tr>
<td>Wall permability</td>
<td>$f_w$ **2.8e-13 m$^2$</td>
</tr>
<tr>
<td>Depth filtration permability</td>
<td>$f_{sd}$ 3.5e-14 m$^2$</td>
</tr>
<tr>
<td>Depth filtration threshold</td>
<td>$\rho_{sd}$ 0.142 kg/m$^3$</td>
</tr>
<tr>
<td>Inlet loss coefficient</td>
<td>$\zeta_{in}$ 1.5 [32]</td>
</tr>
<tr>
<td>Outlet loss coefficient</td>
<td>$\zeta_{out}$ 2.0 [32]</td>
</tr>
<tr>
<td>Sublayer thickness</td>
<td>$\delta_d$ 0.05 mm</td>
</tr>
<tr>
<td>Length of DPF inlet/outlet plugs</td>
<td>$l_{plug}$ 0.01 m</td>
</tr>
</tbody>
</table>

* later changed to 2.1e-14 m$^2$

** later changed to 1.2e-12 m$^2$ for the NC DPF model,
and to 1.5e-13 m$^2$ for the CDPF model

Table 5.3: Soot and filter properties

5.1.2.1 Activation energies $E_a$ and prefactors $K$

In the work by (Cordtz, 2011) [12] activation energies of soot regeneration reactions were found for the NC DPF based on the measured soot burn rates and gas conversions of $NO_2$ and $CO$. The activation energies and pre-factors were provided by fitting simulations with the experimental soot burn rates for the individual regeneration reactions, and the values obtained are used as an initial foundation for the CDPF model, and are seen in table 5.4.
### 5.1.3 Corrected differential pressures in AVL BOOST v2010 in accordance to v5.1

In AVL BOOST v5.1 there was an error in the code for asymmetric channels. A wrong argument was taken when calculating the free outlet channel cross section, and this error has been corrected in v2010. Due to this error the differential pressures in the NC DPF v5.1 model does not correspond as well to the simulated results in v2010 when using the permeabilities fitted by (Cordtz, 2010/2011) [11, 12].

In a Chemical Engineering Journal from 2009, ref.[23], a code was developed in Fortran 77 to simulate both coated and uncoated particulate filters, and they found the following wall permeabilities:

\[
\text{NC DPF : } f_w = 1.2e - 12 \text{ m}^2 \\
\text{CDPF : } f_w = 1.5e - 13 \text{ m}^2
\]

When inserting this wall permeability into the NC DPF model, and adjusting the soot cake permeability to \( f_{sc} = 2.1e - 14 \text{ m}^2 \) the model presented consistent pressure drops with the experimental results, as seen in fig. 5.3. On that account this soot permeability and the CDPF wall permeability from ref.[23] will be used in the proceeding simulations of the CDPF.

In (Cordtz, 2010) [11] an investigation of the individual pressure drop contributions of the overall simulated pressure drop relative to soot mass revealed that the only variable pressure drop, once the initial heating and deep bed filtration regime is passed, is the cake pressure drop. Therefore it was suggested that the discrepancy of the simulated and experimental pressure drop, as seen in fig. 5.4, is related to the soot properties of the cake regime and more specific the soot cake permeability.

**Table 5.4:** Activation energies and pre-factors for the regeneration reactions (Cordtz, 2010) [11]
5.1 CDPF model calibration

5.1.4 O2-NO2 Regeneration Model, soot burn rate and pressure drop

In the BOOST regeneration model it is possible to distinguish between thermal and catalytic soot oxidation, and the O2-NO2 Regeneration Model comprises only thermal soot oxidation, thus the effect of the catalytic coating is not implemented. The soot and filter parameters, activation energies and pre-factors, table 5.3 and 5.4, were implemented in the CDPF model, as specified in the former section, and the result is presented in fig.5.5 and 5.6, which show the measured and simulated soot burn rates and pressure drops respectively. The simulation results agree better with the experimental results than anticipated, even without catalytic kinetics, and the satisfying results is a good confirmation of the activation energies and pre-factors found by (Cordtz, 2011) [12].

The soot kinetics in the model has not been modified to fit a catalytical CDPF, yet the results corresponds to the measured CDPF results. If the improved regeneration for the CDPF was caused mainly by the coating, the BOOST O2-NO2 regeneration model should have shown a curve for the soot burn rate below the experimental results, such that adding the contribution from the catalytical coating would be necessary to achieve the experimental soot burn tendency with the model. Since the simulated and experimental results of the CDPF agree with the O2-NO2 regeneration model it is unlikely that an effect of the catalytical coating is the primary cause of the increased regeneration for the CDPF. There is, however, a small difference in the measured and simulated soot burn rates in test 5, $T_{CDPF} = 444^\circ\text{C}$, where the catalyzed $NO_2$ conversion seems to have a moderate influence on the soot oxidation. The measured $NO_2$ production over the CDPF at this
temperature was high, ~30%, and remarkably higher than the NO\textsubscript{2} production in test 4, \( T_{\text{CDPF}} = 411^\circ\text{C} \), which was measured as less than 10%. The effect of the produced NO\textsubscript{2} in test 5 is less than expected, and it should be mentioned that there are other possibilities for the disagreement in the experimental and simulated soot burn rates at this temperature, other than a contribution of the additional NO\textsubscript{2}. E.g. since the soot burn rate develops exponentially with temperature, just a small adjustment in temperature

![Figure 5.5: Simulated and measured average soot burn rates of CDPF (O2-NO2 Regeneration Model)](image)

![Figure 5.6: Simulated and measured differential pressures (O2-NO2 Regeneration Model)](image)
could give correlated soot burn rates.

The simulated differential pressures fits very well with the measured pressures. There are small differences between the simulated and the measured results in test 4 (engine power = 60%) and 5 (engine power = 67%). In test 5 the simulated pressure drop is higher than the measured, and the experimental results presents a steeper negative gradient than the simulation results both for test 4 and 5. The same tendency was also noticed in the NC DPF simulations, fig. 5.3. Where the pressure drop is both higher and with a steeper slope for the NC DPF test 7 (engine power = 73%).

5.1.5 O2-NO2-NO2-catalytic Regeneration Model, soot burn rate and pressure drop

In the preceding section four regeneration reactions, table 5.1, were applied for the simulation of DPF soot regeneration. These four soot reactions can be extended by an additional reaction to simulate the catalytic oxidation of nitric oxide to nitrogen dioxide, reaction 5 in table 5.1, which takes into account the reversible behavior of the reaction. In coated DPFs this reaction theoretically increases the performance of the NO2-regeneration by reverting NO to NO2, hence increasing the soot burn rate.

The simulated soot burn rates and pressure drops with the O2-NO2-NO2-catalytic regeneration model are presented in fig. 5.7 and 5.8 respectively. As seen the soot burn is correlated with the experimental results for test 5, $T_{CDPF} = 444^\circ C$, without affecting the soot burn rates at the lower temper-

![Figure 5.7: Simulated and measured average soot burn rates of CDPF (O2-NO2 and O2-NO2-NO2-catalytic Regeneration Model)](image-url)
Chapter 5. Simulation Models and Analysis

Figure 5.8: Simulated DPF differential pressures (O2-NO2 and O2-NO2-NO2-catalytic Regeneration Model)

Atmospheres noticeably, this is ensured by choosing a high activation energy. The pressure drop over the CDPF is still correlated to the experimental results, and the frequency factor and activation energy for the NO2-catalytic regeneration reaction are viewed in Table 5.5.

<table>
<thead>
<tr>
<th>Reaction No</th>
<th>K [m^{1.5}/kmol^{0.5}s]</th>
<th>E_a [J/mol]</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>3e32</td>
<td>4.1e5</td>
</tr>
</tbody>
</table>

Table 5.5: Frequency factor and activation energy for the NO2-catalytic regeneration reaction

5.1.6 Catalytic wall reaction, oxidation of CO, HC, NO

For the modeling of the oxidation of nitrogen dioxide, carbon monoxide and hydrocarbons a catalytic wall reaction is added to the model, while the regeneration reaction rates are the same. There are four pre-defined CDPF Catalytic Reactions in BOOST; oxidation of NO, CO, C_3H_6 and C_3H_8. The latter is not relevant in this case, thus only reaction 1, 2 and 4 in the reaction scheme viewed in Table 5.6 is applied. The reactions are assumed to take place in the catalyzed wall in the DPF independently of the presence of soot, hence they do not provide additional reducing agents for the regeneration.
Table 5.6: BOOST CDPF Catalytic Wall Reactions, Oxidation of CO, HC and NO

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Reaction rate</th>
</tr>
</thead>
<tbody>
<tr>
<td>$CO + \frac{1}{2}O_2 \rightarrow CO_2$</td>
<td>$\frac{K_1 y_{CO}^L y_{O2}^L}{D}$</td>
</tr>
<tr>
<td>$C_3H_6 + \frac{9}{2}O_2 \rightarrow 3CO_2 + 3H_2O$</td>
<td>$\frac{K_1 y_{C3H6}^L y_{O2}^L}{D}$</td>
</tr>
<tr>
<td>$C_3H_8 + 5O_2 \rightarrow 3CO_2 + 4H_2$</td>
<td>$\frac{K_1 y_{C3H8}^L y_{O2}^L}{D}$</td>
</tr>
<tr>
<td>$NO + \frac{1}{2}O_2 \rightarrow NO_2$</td>
<td>$K_4 (c_{NO}^L)^2 \cdot c_{O2}^L \cdot \left(\frac{K_4}{K_{eq}} \cdot (c_{NO_2}^L)^2\right)$</td>
</tr>
</tbody>
</table>

Where the following are defined by ref. [9]:

$$D = T_{solid} \cdot \left(1 + K_2 \cdot y_{CO}^L + K_3 \cdot y_{C3H6}^L\right)^2 \cdot \left(1 + K_4 \cdot (y_{CO}^L)^2 \cdot (y_{C3H6}^L)^2 \right) \cdot \left(1 + K_5 \cdot (y_{NO}^L)^0.7\right)$$

(5.10)

$$K_i = k_i \exp\left(-\frac{T_{A,i}}{T_{solid}}\right)$$

(5.11)

$$K_4 = k_4^0 \cdot T_{solid}^4 \exp\left(-\frac{T_A}{T_{solid}}\right)$$

(5.12)

$$K_{eq} = \left(\frac{p_{atm}}{RT_{solid}}\right)^{-0.5} \exp\left(-9.259 + \frac{6848}{T_{solid}} + 0.2791 \cdot \frac{T_{solid}}{1000}\right)$$

$$-0.002245 \left(\frac{T_{solid}}{1000}\right)^2 - 0.4139 \cdot \log\left(\frac{T_{solid}}{1000}\right)$$

(5.13)

The entire wall height is assumed to be catalytically active, and the reactions are activated in all DPF coating sections, meaning they are active through the entire effective length of the DPF monolith. BOOST offers a set of suggested values for the $K_1$-$K_5$ and the activation temperatures $E_1 - E_5$ for the oxidation reactions. These are tuned to fit the measured conversion rates, and the correlated frequency factors and activation temperatures are listed appendix A.2.1.
The simulated species conversions with the catalytic wall reaction applied to the code, are in good agreement with the experimental results, fig. 5.9. In particular the \( NO_2 \) conversion corresponds well at the higher temperatures. The simulated \( NO_2 \) conversion at the lowest test temperature (test 1, \( T_{CDPF} = 305^\circ C \)) on the other hand deviates from the experimental data. An \( NO_2 \) reduction was measured at this temperature, but the cause of this reduction is unclear. The exact magnitude of this \( NO_2 \) conversion could not be obtained with the NO-oxidation mechanisms in BOOST without affecting the \( NO_2 \) production at higher temperatures.

![Figure 5.9: Simulated and measured CDPF species conversions with a catalytic wall reaction applied to the simulation model](image)

**Figure 5.9:** Simulated and measured CDPF species conversions with a catalytic wall reaction applied to the simulation model
5.1.7 Discussion/evaluation of the CDPF model and the BOOST regeneration approach

The CDPF model compare abundantly with the experimental results, with regards to differential pressure, soot burn and species conversions. The activation energies and pre-factors for the thermal soot oxidation reactions from the NC DPF model calibrated by (Cordtz, 2011) [12] was implemented in the CDPF model without modifications, which supports the credibility of both models. It was found that the benefit of the coating was of minor importance when looking at the soot burn rate.

5.1.7.1 Simulated DPF differential pressures

By comparing simulated and experimental DPF pressure drops of the NC DPF and the CDPF series it is found that the results starts to differ at a situation close to where stored and burned soot mass rates are the same. The calibrated models over-estimates the DPF pressure drop. The reason for this behavior is unclear, but it is concluded that something changes in the stored soot structure/distribution, when the DPF model changes from loading to regeneration. Possible explanations are:

- Fast soot burn in depth layer
- Increased soot permeability
- Uneven soot burn rates in DPF

The first option, fast soot burn in depth layer, is relevant when dealing with a catalytic CDPF. Due to the presence of the coating the soot might burn faster in the depth layer compared to the cake layer. If this is the case this could lead to a more “open” structure of the depth layer, depending on the rate of soot transported from the cake layer to the depth layer. However, since the NC DPF model also differ from the experiments it is not believed that the presence of the coating is the controlling mechanism.

The second option, increased soot permeability, concerns the option that the soot layer undergoes a transformation from a packed to a more porous layer when ”entering” the regeneration mode. The theory is that due to the presence of \( O_2 \) and a high temperature the burning of the soot is more uncontrolled and cavities and cracks might develop inside the soot layer, but are not refilled with soot form the inlet channel. Cracks and cavities is a 3D phenomena, something the BOOST code cannot consider.

The third option, uneven soot burn rates in DPF, considers the fact that the DPF core temperature is higher than the outer regions. It is possible
that the soot burn rate is somewhat higher in the core and therefore lead
to an uneven soot distribution throughout the DPF volume. How such an
effect influences the overall pressure drop is not easy to investigate since the
BOOST code does not consider radial changes in soot mass.

5.1.7.2 CDPF Model temperature dependency

As mentioned the temperature is an essential parameter in the DPF regen-
eration model. Instantly the assumption of a mean temperature as inlet BC
in the BOOST model appears to be a reasonable assumption, since higher
inlet temperatures would lead to higher soot burn, which would draw the
simulated results further from the experimental results.

In fig. 5.10 the soot burn rate is presented from simulations with three dif-
ferent DPF inlet temperatures; the measured DPF inlet temperature, the
measured DPF outlet temperature and the mean temperature. As seen the
temperature has a huge influence on the soot burn rate, and especially at
higher temperatures, and a correct temperature is needed to fit the kinetics
of the reactions.

In the BOOST DPF regeneration modes mean values and integrals over
the entire effective DPF length is used to describe the soot layer in the
calculations. Thus it is reasonable to insert the mean temperature, since
that is likely the temperature affecting the average part of the soot layer.
Moreover the simulated and the measured soot burn rates corresponds well
with the mean temperature as model inlet boundary.

With the current CDPF model a minimum monolith size for retrofitting

![Figure 5.10: \( P_{T_{\text{burned}}} \) simulated with CDPF inlet, outlet and mean temperature](image)
a DPF in a larger engine can be determined from the maximum allowed engine back pressure. However, if the CDPF monolith have to be much larger than the tested CDPF the assumption of adiabatic temperature distribution might become invalid.

5.1.7.3 CDPF model O₂-sensitivity analysis

There is a larger uncertainty regarding the O₂ and H₂O concentrations than the other species, as these are calculated from several assumptions, seen in A.1, rather than being logged during the experiments. To determine the importance of the O₂ content a sensitivity analysis was preformed with the BOOST CDPF model by varying the O₂ value in each test, keeping the remaining parameters constant. The H₂O amount is altered to fit the concentration of O₂, and the remaining boundary conditions are taken from the CDPF experimental results. Only simulations with boundary conditions from the three CDPF test with the highest temperatures, test 3-5 table A.1, A.2 appendix A.1 are illustrated.

In fig.5.11 the O₂ percentage is illustrated as a function of the soot burn rate. For test 3 and 4, T_{CDPF} = 383/411°C, the soot burn is practically not influenced by the O₂ concentration. First in test 5, where the gas temperature in the CDPF was as high as 444°C, the soot burn rate shows an increase with increasing O₂ amount, however, the change is small. O₂ ± 0.5%, which is considered the maximum uncertainty regarding the estimated value, contributes to a total change in soot burn rate of less than 0.3 g/h. Hence the O₂ concentration does not have major influence on the simulation results, and the applied calculation method is adequate.

![Figure 5.11: O₂ sensitivity analysis](image)
5.1.7.4 O2-NO2-NO2-catalytic Regeneration Model

For the highest test temperature, the simulated soot burn rate was slightly lower than the measured soot burn. Hence an NO2-catalytic regeneration reaction, section 5.1.5, was added to the thermal soot reactions to increase the soot oxidation by providing additional NO2 as a reducing agent for the regeneration. This seems reasonable because a high NO2 concentration was measured at the CDPF outlet. However, the effect of the additional NO2 was lower than expected, and other aspects could be the cause of this small difference, such as:

- Measured temperature
- Cerium in the coating
- Calculated O2 concentration

Considering the uncertainties regarding the temperatures in the soot layer, fig. 5.10, it is not guaranteed that the additional NO2 formed by the catalytic coating is reacting with the soot and causing higher soot oxidation. Moreover the catalytic coating on the CDPF contains cerium, which may have the ability to lower the O2-reaction temperature, [16]. Since cerium is not implemented in the model the possibility that a more active O2-regeneration is present in real life than what is simulated, cannot be excluded.

Since the O2 concentration was logged during the experiments, but calculated from the air-fuel ratio based on classical diesel cycle assumptions this presents some uncertainties regarding the O2 inlet boundary in the BOOST model. From the O2 sensitivity analysis fig. 5.11 the calculation method was evaluated to be adequate, as the influence of a small change in O2 inlet concentration on the soot burn rate was marginal. However, at the highest test temperature (444°C) the O2 concentration slightly affected the soot burn rate, which can contribute to a deviation between the measured and simulates soot burn rates at this temperature.

5.1.7.5 NO-Oxidation Regeneration

Catalytic wall reactions were calibrated in the CDPF model from the experimental data, and overall the simulated and measured species conversions were in good agreement.

The simulated NO2 conversions matched the measured conversions at the higher temperatures, but for the lowest temperature in the test series (test 1, $T_{CDPF} = 305{^\circ}C$) the simulated NO2 conversion differed somewhat from the
5.1 CDPF model calibration

measured conversion. At this temperature an $NO_2$ reduction was measured. The measured $NO_x$ concentration was more or less equal at CDPF inlet and outlet, fig. 4.12, thus only the reversible NO-NO2 reaction can be responsible for the measured $NO_2$ reduction, but this is not in agreement with the NO-oxidation mechanisms in BOOST. However, a small reduced $NO_2$ concentration could be obtained, and the exact magnitude of this reduction has minor importance for the purpose of this thesis.

5.1.7.6 CDPF simulations with variable initial soot mass

In section 4.1 the influence of the initial soot mass in the DPF on the soot burn rate was discussed. With simulations, this correlation can be further investigated, and this is done by running a CDPF model with initial soot mass as a variable parameter, keeping all other boundary conditions constant. The boundary conditions are taken as the experimental values from the CDPF tests, table A.1 and A.2, with initial soot mass from 0-8 kg/m$^3$ DPF.

The results are seen in figure 5.12 where the measured soot burn rate is plotted versus the measured initial soot mass for reference. As seen the DPF soot mass has a large influence on the soot oxidation, and a different initial soot mass in the first CDPF test would potentially affect the soot burn curve for the entire tested temperature range (305-444°C). It can also be seen that a regeneration of the DPF during a series of tests can affect the exponential growth of the curve.

![Figure 5.12: Simulated $P_T$ burned for various DPF soot masses](image_url)
5.1.8 Investigation of DPF regeneration opportunities

The main challenges associated with DPFs is the regeneration of the soot retained in them. In this section the calibrated DPF model will be applied for the purpose of investigating two different regeneration opportunities; rapid regeneration based on oxidation by oxygen and continuous regeneration based on nitrogen dioxide.

5.1.8.1 O₂ based regeneration triggered by idle gas conditions

If the exhaust conditions allow it passive regenerating systems are possible to use. For all other cases different active regenerating systems are available for rapidly oxidizing the soot trapped in the DPF. In this section it will be investigated if it is possible to regenerate the DPF rapidly without any additional components. To accomplish a rapid regeneration oxygen and temperature are decisive parameters. At engine idle the gas flow is low and the O₂ concentration high, which is ideal regeneration conditions at high temperatures, however, the idle gas temperature is low. If the engine, the exhaust gas and the DPF is preheated to a high temperature, it is possible that a rapid regeneration can take place when the engine load is instantly switched off and the heated DPF is provided with idle gas containing a high O₂ concentration. Idle diesel exhaust gas contains just a few per cent less oxygen than normal air, approximately 18%.

The O₂-regeneration needs high temperatures for activation. In ref.[8] it was seen that the O₂-regeneration is inactive below 400°C and most active between 550 and 600°C, and according to ref. [16] exhaust temperatures above 550°C are required for soot oxidation by O₂. Thus the CDPF inlet temperature is set to 550°C. The idle gas temperature is set to 200°C and initial solid temperature is equivalent to the inlet temperature. At full load the oxygen content in the diesel exhaust is usually near 4%, and as an assumption the O₂ concentration is set to 6% during loaded engine exhaust conditions.

<table>
<thead>
<tr>
<th>Gas properties</th>
<th>Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>m_{soot,init} \ kg/m^3_{DPF}</td>
<td>CO₂ ppm</td>
</tr>
<tr>
<td>P_{DOC,out} \ Pa</td>
<td>CO %</td>
</tr>
<tr>
<td></td>
<td>HC ppm</td>
</tr>
<tr>
<td></td>
<td>O₂ %</td>
</tr>
</tbody>
</table>

Table 5.7: Boundary conditions for the O₂-regeneration simulation model
The total simulation time is set to 20 min, with 1 sec time-step. The constant boundary conditions defined for the model are seen in table 5.7 and are taken as the approximate mean values from the CDPF tests, appendix A.1, except the initial soot mass which is set to 6 and 10 kg\text{soot}/m\textsuperscript{3} DPF. Gas flow, soot concentration, temperature and oxygen concentration, are specified with different values at given time for gas with high engine load and for idle gas as seen in table 5.8.

![Graph](image)

**Figure 5.13:** Inlet and mean DPF temperature during simulation with constant engine load with high inlet temperature ($T_{in} = 550^\circ C$) and stepwise load followed by idle ($T_{in} = 200^\circ C$)
The mean and the inlet temperature for the simulations with the two different initial DPF soot concentrations are equal, and follow the stepwise pattern seen in fig. 5.13. The first engine idle condition is initiated after 2 min. The mean DPF temperature is presented in the upper plot in fig. 5.13, and it is interesting to see that even though the inlet temperature has dropped after two min, the mean temperature has an increasing peak for the simulation with the highest initial soot mass. Which means that a reaction in the DPF is causing the temperature to rise even if the temperature of the gas supplied to the DPF is lower. With $6 \, \text{kg}_{\text{soot}}/\text{m}^3_{\text{DPF}}$ the temperature is decreasing linearly in the DPF and a temperature increase triggered by the idle gas conditions is not seen. The second time engine idle is initiated in the test with $10 \, \text{kg}_{\text{soot}}/\text{m}^3_{\text{DPF}}$ the peak in temperature is not seen either, indicating that it is not enough soot present in the filter to initiate the severe reaction seen the first time.

The overall DPF soot mass is presented in fig. 5.14, and as seen a rapid $O_2$-based regeneration can be achieved if the DPF soot mass is sufficient. With $550^\circ C$ and $10 \, \text{kg}_{\text{soot}}/\text{m}^3_{\text{DPF}}$ (approximately 8 after 2 min when the idle gas is supplied) the DPF regeneration to $3 \, \text{kg}_{\text{soot}}/\text{m}^3_{\text{DPF}}$ is achieved within a minute. With initial soot mass $m_{\text{soot, init}} = 6 \, \text{kg}_{\text{soot}}/\text{m}^3_{\text{DPF}}$ the rapid regeneration is unsuccessful, since a regeneration can be obtained just as fast by keeping steady state conditions, $T(0)-T(20)=550^\circ C$.

![Figure 5.14: DPF soot mass during simulation with constant engine load with high inlet temperature ($T_{in} = 550^\circ C$) and stepwise load followed by idle ($T_{in} = 200^\circ C$)](image)

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5.1 CDPF model calibration

An additional simulation was run, with inlet temperature $T_{\text{in}} = 500^\circ$C and initial soot mass $m_{\text{soot, init}} = 10 \text{ kg soot/m}^3_{\text{DPF}}$ to see if it is possible to obtain the rapid $O_2$-based regeneration at lower temperatures. The inlet and mean DPF temperature are seen together in fig. 5.15. There is no peak in DPF temperature when idle exhaust gas is provided to the DPF, which indicates that the temperature is inadequate to trigger a severe regeneration. As seen in fig. 5.16 regeneration with constant engine load providing an inlet temperature of $T(0)-T(20)=500^\circ$C is in this case more efficient than the induced $O_2$ based regeneration approach.

![Figure 5.15: Inlet and mean DPF temperature during simulation with constant engine load with high inlet temperature ($T_{\text{in}} = 500^\circ$C) and stepwise load followed by idle ($T_{\text{in}} = 200^\circ$C)](image1)

![Figure 5.16: DPF soot mass during simulation with constant engine load with high inlet temperature ($T_{\text{in}} = 500^\circ$C) and stepwise load followed by idle ($T_{\text{in}} = 200^\circ$C)](image2)
5.1.8.2 \( \text{NO}_2 \) supported continuous regeneration

It is important to keep the engine back-pressure as low as possible, especially in auxiliary engines where the fuel consumption is high. Retrofitting a DPF will cause a higher engine back-pressure, and it is important to make sure that the back-pressure is within an acceptable level, and as low as possible to prevent the fuel consumption from increasing noticeably. Continuous regeneration of the DPF, such that the soot mass is relatively low at all times, will reduce the DPF pressure drop, hence the back-pressure, and the necessary size of the DPF monolith.

\( \text{NO}_2 \) oxidizes soot at reasonable rates at temperatures as low as 250\(^\circ\)C, \cite{16}, therefore continuous \( \text{NO}_2 \) based regeneration strategies is investigated for the DPF. The CDPF test results, A.1, are used to define the boundary conditions for the model seen in table 5.14. The soot concentration is defined as the highest measured in the test while mean values are approximated for the remaining boundaries. The \( \text{NO}_x \) concentrations measured in the CDPF tests, were taken as an approximate for the maximum available \( \text{NO}_2 \) at the DPF inlet. Whether it is realistic to assume that all the \( \text{NO} \) can be oxidized to \( \text{NO}_2 \) will not be considered, neither will possibilities of providing additional \( \text{NO}_2 \). The rounded measured \( \text{NO}_x \) concentrations and temperatures are seen in table 5.10.

<table>
<thead>
<tr>
<th>Gas properties</th>
<th>Species</th>
</tr>
</thead>
<tbody>
<tr>
<td>PM(<em>{\text{in}}), ( \text{G}</em>{\text{exh, in}} ), ( \text{P}_{\text{DOC, out}} )</td>
<td>CO(_2), CO, H(_2)O, HC, O(_2)</td>
</tr>
<tr>
<td>- kg/h Pa</td>
<td>% ppm % ppm %</td>
</tr>
<tr>
<td>0.3e-4 180 112500</td>
<td>8.0 150 8.0 22 9.0</td>
</tr>
</tbody>
</table>

Table 5.9: Boundary conditions for the \( \text{NO}_2 \)-regeneration simulation model

<table>
<thead>
<tr>
<th>Test no</th>
<th>Load %</th>
<th>( T_{\text{CDPF, in}} ) (^\circ)C</th>
<th>( \text{NO}_x ) ppm</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>37</td>
<td>300</td>
<td>750</td>
</tr>
<tr>
<td>2</td>
<td>45</td>
<td>350</td>
<td>900</td>
</tr>
<tr>
<td>3</td>
<td>52</td>
<td>380</td>
<td>1300</td>
</tr>
<tr>
<td>4</td>
<td>60</td>
<td>410</td>
<td>1800</td>
</tr>
<tr>
<td>5</td>
<td>67</td>
<td>450</td>
<td>1700</td>
</tr>
</tbody>
</table>

Table 5.10: Rounded measured temperatures and \( \text{NO}_x \) concentrations from the CDPF tests

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It was seen from the experiments that no noteworthy oxidation is happening below 300°C, and according to references [8, 11] the O₂ supported regeneration is inactive below 400°C, and once the O₂ oxidation is initiated it is likely to dominate the regeneration reactions as the O₂ concentration is 2-3 orders of magnitude higher than the NO₂ concentration. Thus the temperature range that will be investigated is 3-400°C, where the NO₂ regeneration is expected to be dominant. The NO concentration is set to zero, since the assumption is that all available NO is oxidized to NO₂ upstream the DPF, thus the catalytical coating on the DPF has no influence on the regeneration.

First a short simulation, 1h simulation time, with output every time-step of 25 sec, is run with the purpose of identifying the necessary NO₂ inlet concentration for continuous regeneration of the DPF. The overall DPF soot mass is observed, and when the soot mass is in equilibrium, continuous regeneration is achieved. Initially a clean filter was tested, however, with a clean filter and only one hour simulation time an NO₂ concentration of 2\% was necessary to maintain continuous regeneration, which means that it is not possible to keep the filter entirely clean. Soot has to be captured in the filter for the initiation of the regeneration. Therefore three different initial soot masses were investigated, and the minimum NO₂ amount to obtain a soot mass equilibrium point for the different soot masses is seen in table 5.11, and it is clear that the temperature and the soot mass have large influence on the regeneration.

<table>
<thead>
<tr>
<th>m_{soot,init} kg/m³_{DPF}</th>
<th>T_{DPF, in} °C</th>
<th>NO₂_{in} ppm</th>
<th>Theoretical Max NO₂ ( \leq NO_x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>400</td>
<td>20000 (2%)</td>
<td>above</td>
</tr>
<tr>
<td>2</td>
<td>300</td>
<td>2290</td>
<td>above</td>
</tr>
<tr>
<td>2</td>
<td>400</td>
<td>1200</td>
<td>ok</td>
</tr>
<tr>
<td>3</td>
<td>300</td>
<td>1500</td>
<td>above</td>
</tr>
<tr>
<td>3</td>
<td>400</td>
<td>780</td>
<td>ok</td>
</tr>
<tr>
<td>5</td>
<td>300</td>
<td>880</td>
<td>above</td>
</tr>
<tr>
<td>5</td>
<td>400</td>
<td>460</td>
<td>ok</td>
</tr>
</tbody>
</table>

Table 5.11: NO₂ concentrations necessary to obtain continuous regeneration within 1h simulation time

From table 5.11 it is seen that at 300°C a higher soot mass or a higher NO₂ amount than the measured NOₓ concentration, table 5.10, is required. Continuous regeneration is a time consuming process, and longer simulation...
time is necessary. It is not impossible that continuous regeneration can be achieved with 300°C given long enough time, however, due to the poor performance seen in table 5.11 300°C is not considered further in this study.

The time needed to obtain an equilibrium soot mass is further studied for the three $NO_2$ concentrations seen for 400°C inlet temperature in table 5.11. An initially clean filter will be simulated, with 10h simulation time. During the CDPF experiment steady state conditions were reached after approximately 20 min, hence the first 20 min of the simulation will have a linear increase in temperature and $NO_2$, $(T(0)=0°C, NO2(0) = 0$ppm), with temperature from 0-400°C as seen in fig. 5.17. The overall DPF soot mass is also seen in the figure, and with 1200 ppm $NO_2$ an equilibrium soot mass of 2 kg/m$^3$$_{DPF}$ is seen after approximately 6h, and with 780 ppm $NO_2$ the soot mass seems to be approaching equilibrium state, however, with the lowest $NO_2$ concentration, 460 ppm, a noticeable increase in soot mass can be observed.

![Figure 5.17: DPF soot mass and inlet temperature during 10 hour $NO_2$-regeneration simulation](image)

Continuous regeneration during 24h is investigated. Auxiliary engines are usually operated with fixed rpm, unlike vehicles where the engine rotational speed in continuously varying, and they are likely to be ran for several hours at this fixed rpm, before they are turned off. A stepwise simulation is run order to see the influence of switching of the engine, thus loading the filter
5.1 CDPF model calibration

![Graph showing DPF soot mass and inlet temperature during 24 hour NO\textsubscript{2} regeneration simulation. Dashed line shows simulation with constant temperature after 20 min and solid line with the temperature progress seen in the bottom figure.]

Additionally during the 20 min heating period when starting the engine. The engine is thought started and ran at a fixed engine load in 8h intervals with 20min soot loading each time during 24h, as seen from the transient inlet temperature in fig. 5.18.

From the overall DPF soot mass in fig. 5.18 it is seen that after 24h an equilibrium soot mass is obtained for all the tested NO\textsubscript{2} inlet concentrations, and regardless of additional soot loading the soot mass will come in balance after few hours regeneration at the same soot amount depending only on the NO\textsubscript{2} inlet concentration. The time spent before the soot mass equilibrium is reached varies with the NO\textsubscript{2} amount. With 1200 ppm NO\textsubscript{2} equilibrium was seen after approximately 6h and it was seen after 14h with 780 ppm, and for the test with the less NO\textsubscript{2} amount, 460 ppm, it took all 24h to reach an approximate equilibrium soot mass.

From this investigation it can also be observed that rapid NO\textsubscript{2} supported regeneration is not particularly relevant, since this presumably will demand unrealistically high NO\textsubscript{2} concentrations.
5.2 DOC model calibration

The BOOST CAT code calculated the gas dynamic performance of the catalyst as well as the pressure drop over the catalyst depending on the actual flow conditions.

If the chemical reactions are not activated the catalyst is understood as a flow element where only data about geometry and friction is required. The BOOST CAT model offers several different reaction models. Either no reactions are taken into account, pre-defined reaction models are chosen or the application of user defined models is possible.

5.2.1 DOC Reaction model (Conversion reactions)

The BOOST DOC reaction model comprises three major oxidation reactions of CO, HC, and NO. The reactions are of the Longmuir Hinselwood type and are viewed in table 5.12. The rate equation and a set of suggested values of all parameters are given.

<table>
<thead>
<tr>
<th>Rate equation</th>
<th>Stoichiometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>R1</td>
<td>CO + 1/2 O₂ → CO₂</td>
</tr>
<tr>
<td>R2</td>
<td>C₅H₆ + 9/2 O₂ → 3CO₂ + 3H₂O</td>
</tr>
<tr>
<td>R3</td>
<td>2NO + O₂ ↔ 2NO₂</td>
</tr>
</tbody>
</table>

Table 5.12: DOC conversion reactions

The rate equations for the oxidation of carbon monoxide and hydrocarbons are given as

\[
R1 = \left( \frac{K_1 \cdot e^{-E_1/RT_s} \cdot y_{CO} \cdot y_{O_2}}{1 + K_4 \cdot e^{-E_4/RT_s} \cdot y_{CO}^2 \cdot y_{C_3H_6}} \right) \cdot \left[ 1 + K_2 \cdot e^{-E_2/RT_s} \cdot y_{CO} + K_3 \cdot e^{-E_3/RT_s} \cdot y_{C_3H_6} \right]^{-2} \cdot T_s
\]

(5.14)

\[
R2 = \left( \frac{K_1 \cdot e^{-E_1/RT_s} \cdot y_{C_3H_6} \cdot y_{O_2}}{1 + K_4 \cdot e^{-E_4/RT_s} \cdot y_{CO}^2 \cdot y_{C_3H_6}} \right) \cdot \left[ 1 + K_2 \cdot e^{-E_2/RT_s} \cdot y_{CO} + K_3 \cdot e^{-E_3/RT_s} \cdot y_{C_3H_6} \right]^{-2} \cdot T_s
\]

(5.15)
where the frequency factors $K_n$ and the activation temperatures $E_n$ can be adjusted by the user.

For the reversible oxidation of nitric oxide and nitrogen dioxide two different rate approaches can be chosen. In this report only Rate approach 1, which is shown in table 5.12 is used. The rate equation for this NO-oxidation is given

$$R3 = K \cdot T_s^A \cdot e\left(\frac{-E}{T_s}\right) \cdot \left[\frac{2}{K_{Equ,1}(T_s)} \cdot c_{NO} \cdot c_{O2} - \frac{c_{NO_2}^2}{K_{Equ,1}(T_s)}\right]$$

(5.16)

where the frequency factor $K$, the activation temperature $E$ as well as the temperature dependency $A$ can be adjusted by the user. The temperature dependency is set to 1, and the frequency factors and activation temperatures for the $HC$, $CO$ and $NO$ oxidation are tuned iteratively to fit the experimental results, and are shown in appendix A.2.2.

### 5.2.2 DOC model initiation and boundary conditions

The boundary conditions applied for the DOC model are listed in appendix A.1.2. The inlet boundaries are exhaust temperature $T_{exh}$, mass flux $G_{exh}$ and gas fraction. The only required outlet boundary is the exit pressure $p_{DOC,out}$. Square cell catalyst is chosen as the specification of the honeycomb structure, which means that the hydraulic diameter of the catalyst pipe is defined via the cpsi value and a washcoat thickness seen in table 5.13. The physical properties of the DOC monolith is also seen in the table.

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Monolith volume</td>
<td>0.001634 m$^3$</td>
</tr>
<tr>
<td>Length of monolith</td>
<td>0.1185 m</td>
</tr>
<tr>
<td>Cell Density (cpsi)</td>
<td>300 1/in$^2$</td>
</tr>
<tr>
<td>Wall thickness</td>
<td>0.007 in</td>
</tr>
<tr>
<td>Washcoat thickness</td>
<td>0.0005 in</td>
</tr>
<tr>
<td>Density</td>
<td>1413 kg/m$^3$</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>0.4 W/m K</td>
</tr>
<tr>
<td>Specific heat</td>
<td>1130 J/kg K</td>
</tr>
</tbody>
</table>

*Table 5.13: DOC physical properties*

The DOC is simulated in the aftertreatment analysis mode, hence the specification of a friction coefficient is necessary. BOOST offers predefined turbulent and laminar coefficients, and they are kept at the default values. The simulation is adiabatic and, the discretization is made as a 1D structure with 15 axial grid points, and a grid shape factor 1.
5.2.3 Simulated DOC species conversions and soot burn

Figure 5.19 illustrates the simulated and measured species conversions in the DOC after fitting the frequency factors and activation temperatures. The simulated conversion of CO and HC fits very well with the experimental results. The simulated NO\textsubscript{2} conversions where an NO\textsubscript{2} production was measured is in good agreement with the experimental results. However, an NO\textsubscript{2} production was measured at 313°C, which could not be fitted with the NO-oxidation mechanisms in BOOST.

5.2.3.1 Simulated NO\textsubscript{2} conversion over the DOC

The NO\textsubscript{2} conversion in the DOC is illustrated as a function of temperature in fig. 5.20. The boundary conditions for the simulation is taken as the experimental values from DOC test 4, where the O\textsubscript{2} concentration is 7.28%,
with DOC inlet temperature increasing linearly from 0 to 600°C, during one hour test time. The maximum \( NO_2 \) production is seen at approximately 430°C.

The \( NO \) and \( NO_2 \) are in equilibrium below around 280°C and above approximately 500°C, which means that the DOC does not influence the regeneration in the downstream DPF above 500°C. The equilibrium temperatures depend on the oxygen, and with a higher \( O_2 \) concentration there will be \( NO_2 \) production at higher temperatures, however, not significantly, since the maximum \( NO_2 \) production still will occur at 430°C.

![Simulated \( NO_2 \) conversion over the DOC as a function of temperature](image)

**Figure 5.20**: Simulated \( NO_2 \) conversion over the DOC as a function of temperature

### 5.2.3.2 DOC soot burn expressed empirically

From the experimental results a considerable soot oxidation was measured in the DOC, and this should be accounted for in the CRT (DOC+NC DPF) and CCRT (DOC+CDPF) models, in order to model the overall system soot oxidations. The specific inlet soot concentration \( (mg_{soot}/kg_{EXH}) \) is the only boundary condition in the DPF model that is affected by the soot oxidation in the upstream DOC. Therefore the DOC soot oxidation can be implemented in the model simply by adjusting the soot concentration, thus the following temperature dependent expression was derived for the DOC outlet soot mass concentration:

\[
PMc_{DOC,out} = PMc_{DOC,in} \cdot 1.66 \cdot [3.3 - \ln(1.8 \cdot T_{DOC,in})]
\] (5.17)
In the DOC model soot is implemented as a solid mass fraction in the inlet boundary. The soot is, however, not participant of any reactions in the DOC, the soot mass exiting the DOC is equal to the mass entering the DOC ($PM_{DOC,in} = PM_{DPF,in}$).

Fig. 5.21 shows the measured and the empirically expressed soot burn rate for the DOC.

$$ PM_{measured at DOC outlet} = PM_{expressed by:} $$

$$ PM_{in} \times 1.66 \times (3.3 - \log_{10}(T_{DOC,in} \times 1.8)) $$

**Figure 5.21:** Expressed soot burn rate over the DOC

### 5.2.4 Discussion/evaluation of the DOC model and the soot oxidation approach

A DOC model was successfully calibrated by adjusting the reaction parameters for the oxidation reactions. With exception of the $NO_2$ reduction measured at the lowest test temperature, the conversions of $CO$, $HC$ and $NO$ corresponds very well with the experimental results.

#### 5.2.4.1 DOC soot oxidation approach

The measured soot oxidation in the DOC was implemented in the model by deriving an empirical temperature dependent expression for the outlet soot concentration with respect to the inlet concentration.

In the BOOST CAT model it is possible to define user defined reactions with soot. In this case it is necessary to define soot as surface species. The oxidation reaction in which can be defined is following the same reaction approach as for the soot oxidation in the DPF model, which is why it was
decided not to follow that approach. In a DPF the particles are structured as a soot layer, where the thickness and the permeability of the layer is essential, while properties of the individual particles, such as particle size, on the other hand is less important. In the DOC the particles are not trapped as in the DPF, hence the oxidation of soot has a different nature, where the important parameters are the flow and the particle properties. The particles released from an engine varies a lot, therefore a calibration of the regeneration reactions for a DOC will present a lot of uncertainties. The activation energies does probably not vary much, but the pre-factor is dependent on particle size and the flow, which makes it is difficult to calibrate the model precisely. Also the oxidation is more likely to occur in a porous media, meaning the particle porosity is affecting the probability that reaction occurs. Therefore it was decided that it was better to make an empirical expression for the soot concentration in the flow, such that the model is calibrated precisely for the measured soot concentrations in this experiment, however, it is not claimed to be a general expression for the soot oxidation in the DOC. For presenting a comparison between the after treatment systems, this approach is adequate, as it will take into consideration the soot oxidation measured in the DOC at different temperatures. With this approach will changes in species concentrations due to the reaction mechanisms of the soot oxidation will not be considered.

5.2.4.2 NO-Oxidation Regeneration

The focus in this thesis is the contribution of the DOC in a DPF system with regards to the soot regeneration in the DPF, thus the $NO_2$ conversion is the most essential reaction in the DOC. The simulated $NO_2$ conversions where an $NO_2$ production was measured is in good agreement with the experimental results. However, a reduced $NO_2$ concentration was measured at the DOC outlet at 313°C, which could not be fitted with the NO-oxidation mechanisms in BOOST.

In this work the main purpose of the DOC model is to combine the calibrated model with the DPF models for investigating the soot regeneration, hence the focus is to have a correlated model at the temperatures where noticeable soot oxidation is present in the DPFs. The soot burn rate measured in the CDPF and the NC DPF was insignificant at temperatures near 300°C, therefore the accuracy at this temperature is of small importance. It is, however, important that the model does not produce a higher $NO_2$ concentration, as this could enhance the simulated soot burn rate in a downstream DPF, and produce inaccurate results for the following CCRT and CRT simulations. The missing $NO_2$ reduction at 313°C in the DOC model was concluded to be of small importance as the current conversion produced by the model is
nearly zero. The DOC cannot contribute to an enhanced regeneration at this temperature, and the DOC model will not simulate that either, since the NO-oxidation reaction is nearly inactive. Generally the conversion rates produced by the model agree well with the experimental results.
5.3 CCRT and CRT simulations in BOOST

Modeling the two-brick aftertreatment systems CCRT (DOC+CDPF) and CRT (DOC+NC DPF) is done in BOOST by redefining the individually calibrated models of the DOC and the DPFs in combination. Simply by turning on and off the catalytical wall reaction in the DPF model one can switch between modeling the CCRT and CRT system.

5.3.1 Simulated soot burn rates for CCRT

Figure 5.22 shows the simulated test series with the CDPF, CRT and CCRT models. The boundary conditions applied are the measured properties from the CDPF experiment, appendix A.1. Two different DOC inlet conditions for the exhaust soot concentration $PMc$ have been implemented in the CCRT model: one with the measured $PMc$ at the CDPF inlet and the second with $PMc$ empirically expressed to account for the DOC soot oxidation. The expression (5.17) gives the $PMc$ at the DOC outlet depending on the $PMc$ inlet values and the temperature. In the model reactions with soot is only active in the filter, and the soot entering the DOC equals the soot entering the DPF. With this simplified approach changes in species concentrations due to the reaction mechanisms of the soot oxidation will not be considered, and the model only presents the conversions fitted to the experimental data, in which the soot oxidation is included.

A large improved soot burn is seen in figure 5.22 for the CCRT compared to
the single CDPF, both with and without including the soot oxidation in the DOC. It is apparent that the increased $NO_2$ at the CDPF inlet due to the $NO$-oxidation in the DOC increases the soot burn significantly. The CRT system is only illustrated with the soot oxidation included, and from the comparison of the CCRT and CRT it is apparent that the CDPF coating has an insignificant influence on the soot burn in the CCRT system.

Fig. 5.23 presents the simulated DPF pressure drops with the CCRT model compared to the CDPF model. The pressure drop over the CCRT system is equivalent to the pressure drop over the single CDPF at test 1, $T_{\text{in}} = 305^\circ\text{C}$, before any noticeable soot oxidation is present. Thus it can be concluded that the DOC is not contributing to an additional engine back-pressure. The differences is increasing with further soot oxidation, due to the different soot masses in the CDPF with and without an upstream DOC. From the differential pressure gradients it can be seen that the DPF regeneration is initiated at a lower temperature for the CCRT than the single CDPF, as the gradient is slightly negative in test 3, $T_{\text{CCRT,in}} = 383^\circ\text{C}$ for the CCRT while the gradient for test 3 and 4, $T_{\text{CDPF,in}} = 383, 411^\circ\text{C}$, both are positive with the single-CDPF simulation. Which can indicate that the additional $NO_2$ provided to the CDPF can reduce the temperature where soot oxidation is initiated, however the oxidation rate at this temperature is more affected.
5.3 CCRT and CRT simulations in BOOST

5.3.2 Simulated case for comparing the regeneration and species convergence of the CDPF, CCRT and CRT

In order to compare the single CDPF, the CCRT and the CRT systems a set of average boundary conditions from the tests are applied for the different models. In order to see the influence of changes in temperature and \( NO_2 \) concentrations all other parameters are defined as constants. For all constant parameters an approximately mean value from the experimental tests have been chosen, and the inlet temperature is defined as a linear transient variable from 300-500\(^\circ\)C, and the simulation time is one hour. The simulations are performed with two different \( NO_2 \) concentrations for investigating the influence of the \( NO_2 \) amount on soot burn and species conversions. The \( NO \) concentration is chosen as a function of the \( NO_2 \) concentration, as seen in table 5.14. The initial soot mass in the DPF is set to 5 kg/m\(^3\).

| Variables | | |
|---------|---------|---------|---------|
| Time \( s \) | \( T_{in} \) \( ^\circ \)C | \( NO_2 \) ppm | \( NO \) ppm |
| 0-3600 | 300-500 | 100/300 | 6NO\(_2\) |

| Constants | | |
|---------|---------|---------|---------|---------|---------|---------|
| Gas properties | | Species | | | | |
| PM\(_c,\text{in}\) | \( G_{\text{exh,}\text{in}} \) kg/h | \( p_{out} \) Pa | CO\(_2\) | CO | H\(_2\)O | HC | O\(_2\) |
| 0 | 180 | 112500 | 8.0 | 150 | 8.0 | 22 | 9.0 |

*Table 5.14: BOOST boundary conditions for the simulated case*

5.3.2.1 CDPF, CCRT and CRT differential pressures and soot mass

The overall DPF soot mass in the CDPF, CCRT and CRT models are presented with the two different \( NO_2 \) inlet conditions; 100 and 300 ppm in fig. 5.24. The soot masses are illustrated as a function of time and mean DPF temperature, in the time-range where time and temperature has a linear correlation (10-50 min).

The soot mass is decreasing considerably more for the CRT and the CCRT system than for the single CDPF, while the difference between the two-brick systems is minimal. The improved soot burn in the CRT and CCRT
is noticeably larger with higher \( NO_2 \) concentrations at the inlet. With \( NO_{2,in} = 300 \text{ppm} \) a significant PM to temperature gradient is seen above approximately 400°C and the difference between the CRT/CCRT systems and the single CDPF is approximately five times larger with \( NO_{2,in} = 300 \text{ppm} \) than with \( NO_{2,in} = 100 \text{ppm} \), which means that a sufficient inlet \( NO_2 \) con-

\[ \text{Figure 5.24: Simulated overall DPF soot mass for CDPF, CCRT and CRT with inlet concentration of } NO_2 = 100 \text{ and } 300 \text{ ppm} \]

\[ \text{Figure 5.25: Simulated differential pressure for the CDPF, CCRT and CRT with inlet concentration of } NO_2 = 100 \text{ and } 300 \text{ ppm} \]
centration is essential for utilizing the full potential of the DOC with regards to DPF regeneration.

Figure 5.25 presents the pressure drops over the three DPF systems. The pressure drop is higher over the single CDPF than over the CRT and CCRT systems, which is expected since the soot burn rate is higher for the CRT and CCRT systems. In fig. 5.23 it was seen that at equivalent soot masses the CCRT system pressure drop is equal to the pressure drop over a single CDPF, thus the difference in pressure drop between the CDPF and CRT/CCRT system is caused by differences in the DPF soot mass. The maximum pressures were located at time 50, 51 and 55 min for the CCRT, CRT and CDPF respectively for the simulations with \( NO_{2, in} = 300 \text{ ppm} \) (at the temperatures 469, 470 and 482\(^\circ\text{C} \)).

5.3.2.2 CDPF, CCRT and CRT species conversions

The \( NO_2 \) conversion for the CDPF, CCRT and CRT systems are presented as a function of temperature and time in fig. 5.26. For the CDPF the overall \( NO_2 \) conversion is similar with 100 and 300 ppm \( NO_2 \) inlet concentration, while for the CRT and CCRT systems the \( NO_2 \) inlet concentration influences the conversion rate significantly. The conversion rate is definitely highest for

![Figure 5.26: \( NO_2 \) conversion for the CDPF, CCRT and CRT system with inlet concentration of \( NO_2 = 100 \) and 300 ppm](image-url)
the CCRT system, as expected, however, around 480°C the CCRT and the CDPF curves meet. From this correlation it can mistakenly be interpreted that the DOC will not contribute to a higher soot oxidation in the CDPF at temperatures above ~480°C, however, all the NO\textsubscript{2} produced in the DOC will pass the soot layer in the downstream CDPF, while only some of the NO\textsubscript{2} produced in the CDPF will pass the soot layer, as discussed previously. It can on the other hand be seen from the overall DPF soot mass, fig 5.24, which have equivalent gradients for the three systems above 480°C, that the contribution of the DOC is minimal above this temperature. The slopes are calculated from the first coefficients of the polynomial for the soot mass vectors from \( T = 480 - 500 \)°C to be -1.1 for the two-brick systems and -1.11 for the single CDPF.

The average NO\textsubscript{2} concentrations at system inlet and outlet for the CDPF, CCRT and CRT are illustrated in fig. 5.27. The CDPF clearly has the lowest NO\textsubscript{2} concentration at the outlet, and the high NO\textsubscript{2} emission for the CCRT system apparently is a trade-off for the well improved soot oxidation.

![Average NO\textsubscript{2} concentrations at system inlet and outlet for the CDPF, CCRT and CRT](image)

**Figure 5.27:** Average NO\textsubscript{2} concentrations at system inlet and outlet for the CDPF, CCRT and CRT

Figure 5.28 shows the simulated HC conversion for the CDPF, the CCRT and the CRT systems. The HC reduction is higher for the two-brick systems than for the single CDPF. The HC convergence is increasing with temperature for all three systems, and for the CCRT the convergence is reaching 100% above ~460°C. The HC convergence will not be influenced by the inlet NO\textsubscript{2} concentration, since there is no reactions present where HC reacts with NO\textsubscript{2}. The system CO convergence on the other hand will be influenced by the inlet NO\textsubscript{2} concentration.

The simulated CO conversion for the CDPF, the CCRT and the CRT, with NO\textsubscript{2} inlet concentration of 100 and 300 ppm is illustrated in fig. 5.29. It is interesting to see that the transient CO conversion tends towards zero for
5.3 CCRT and CRT simulations in BOOST

the CRT system. This means that in order to reduce the CO emissions the catalytic coating on the DPF is essential. The CCRT system shows close to 100% CO conversion for the entire plotted temperature range. The CDPF also shows close to 100% convergence depending on the NO$_2$ content. When the NO$_2$ inlet concentration is high, the CO conversion is not more than 80% at 340$°$C, however, it is still approaching 100% at higher temperatures.

Figure 5.28: HC conversion for the CDPF, CCRT and CRT system

Figure 5.29: CO conversion for the CDPF, CCRT and CRT system with inlet concentration of NO$_2 = 100$ and 300 ppm

July 2011

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5.4 Conclusive summary and discussion

A CDPF model, a DOC model and a combination of these for simulating CRT and CCRT systems were successfully calibrated in BOOST.

The influence of the initial soot mass in the DPF on the soot burn rate was investigated with the calibrated CDPF model, and as discussed in chapter 4 the DPF soot mass was seen to have a large influence on the soot oxidation. Which shows that the improved soot burn rate that was measured for the CDPF with respect to the NC DPF needs to be considered with caution, given the higher initial soot mass in the NC DPF tests.

The activation energies and pre-factors for the thermal soot oxidation reactions (NO-NO2 Regeneration Model) from the NC DPF model calibrated by (Cordtz, 2011) [12] was implemented in the CDPF model without modifications, and yet the model produced soot burn rates in agreement with the experimental results. Since the O2-NO2 Regeneration Model comprises only thermal soot oxidation it indicates that the benefit of the coating was of minor importance when looking at the soot burn rate.

The soot kinetics in the model was later modified to fit a catalytical CDPF by using the NO-NO2-NO2-catalytic Regeneration Model in BOOST, however, the correction was small with minor influence on the DPF regeneration. Seen from the comparison of the soot oxidation produced by the CRT and CCRT model, the modification, thus the influence of the catalytic coating, was insignificant. The contribution of the DOC in the DPF system on the other hand was seen to be very effective with regards to the soot oxidation in the downstream DPF, as the CRT and CCRT systems offers significant advantages for the NO2-based DPF regeneration. Additionally the system pressure drop was equal over all systems (CCRT, CRT, CDPF) given the DPF soot mass is the same, thus the DOC does not contribute to a higher engine-back pressure in case of a CRT or CCRT system. The CCRT system shows remarkably higher HC conversions than the CRT system, and it was concluded that in order to remove a sufficient amount of hydrocarbons in the emissions the CDPF is decisive. However, the NO2 emissions from the CCRT systems is higher than the for the CRT system, nevertheless the soot burn is equivalent. Which means that a lower CO emission is on the expense of a higher NO2 emission. Thus it might be relevant to produce catalytical coatings for the DPF that only comprise HC and CO oxidations for use in CCRT systems.

The calibrated DPF model was also used for the purpose of investigating rapid regeneration based on oxidation by oxygen and continuous regeneration based on nitrogen dioxide. It was demonstrated that it is possible to maintain continuous regeneration with adequately NO2 concentrations and temperatures. Dimensioning a DPF for a larger engine is easier if continuous
regeneration can be considered, since the average soot mass then can be determined, and moreover will be rather constant. The temperature of which continuous regeneration was investigated was \( T_{DPF,in} = 400^\circ C \), and with an \( NO_2 \) inlet concentration of 460 ppm a soot mass of \( 5kg/m^3_{DPF} \) could be maintained. Seen from the simulated \( NO_2 \) conversion over the DOC the optimal conversion is located at temperatures around \( T_{DPF,in} = 400^\circ C, \) fig.5.20, and the required \( NO_2 \) amount to maintain a continuous regeneration in this temperature area should be possible to achieve with the DOC. Although higher \( NO_2 \) concentrations would result in a more efficient regeneration, and a lower soot mass balance, thus also a lower engine back-pressure. Hence optimizing DOCs with regards to the \( NO \) oxidation reaction can be the direction to head for further investigation of DPF systems for auxiliary engines. An issue which will have to be addressed regarding the \( NO_2 \) supported continuous regeneration is the high \( NO_2 \) emissions at the DPF outlet. High \( NO_2 \) inlet concentrations gives high outlet concentrations as well, thus in that matter it is an advantage to keep the \( NO_2 \) inlet amount as low as possible, however, lower \( NO_2 \) emissions will be at the expense of higher engine back-pressure.

In auxiliary engines where the fuel consumption is high it is especially important to keep the engine back-pressure as low as possible. Installing a DPF will cause a higher engine back-pressure, and it is important to make sure that the back-pressure is within an acceptable level, and as low as possible to prevent the fuel consumption from increasing noticeably. Continuous regeneration of the DPF, such that the soot mass is relatively low at all times, will reduce the DPF pressure drop, hence the back-pressure, and the necessary size of the DPF monolith. Moreover it is beneficial if the DPF can be designed such that it can do without monitoring.

\( O_2 \) based regeneration triggered by idle gas conditions was also investigated. If the engine, the exhaust gas and the DPF is preheated to a high temperature, (\( \sim 550^\circ C \)), it is possible to trigger an \( O_2 \)-regeneration that will clean the filter in few minutes by supplying gas with idle conditions. The reaction that will occur is so active that, even if the supplied idle gas has much lower temperature, the DPF temperature will continue increasing a short while, due to the soot oxidation. For this reaction to occur it was seen that an adequate DPF soot mass was essential for cleaning the DPF rapidly. This is an interesting study to proceed with, as it allows regeneration without additional components. E.g. can it be used as a safety measure in a continuous regenerating DPF system. In case of a potential system error leading to filter clogging, the filter can be emptied for soot efficiently simply by controlling the engine power in the right matter.
Experiments based on raw exhaust gas sampling was conducted for the purpose of investigating the performances regarding soot oxidation and conversion rates for a coated DPF (CDPF) and a DOC. A DPF model and a DOC model was calibrated separately in AVL BOOST v2010 on the basis of results from the experiments, additionally a combination of the two models were used for simulating the two DPF systems CCRT and CRT.

6.0.1 Conclusions

Effect of catalytic coatings applied in diesel particulate filter (DPF) systems has been the focus. Comparison with in-house experiments on an un-coated filter (NC DPF), has been used for identifying the catalytical contribution of the CDPF coating to the regeneration, and for studying the contribution of an upstream DOC in a DPF system CRT and CCRT simulations has been run.

From the measured balance point temperatures (BPT) and soot burn rates versus temperatures the CDPF results showed, what appeared to be, an improved oxidation of soot, however, when presenting the results with respect to the soot mass and temperature the CDPF and NC DPF results were more resembling. The soot mass is seen to have a large influence on the soot burn rate, and it was concluded that the BPT is an unreliable parameter for comparing the two DPFs due to the influence of physical parameters such as the DPF soot mass and exhaust gas soot- and species concentrations.
The DOC experimental tests showed promising results regarding the DOC performance, considering both species conversion and soot oxidation. Not only does the DOC enhance the soot oxidation in the DPF, a soot reduction of approximately 50% was measured over the DOC at inlet temperature $T_{\text{DOC,in}} \sim 500^\circ\text{C}$.

An $\text{NO}_2$ production of approximately 50% was measured for the DOC at temperatures between 4-500$^\circ\text{C}$, and it was seen that CRT and CCRT systems offer significant advantages for the $\text{NO}_2$-based DPF regeneration, opposed to the CDPF which only showed a small, if any, improved oxidation. The CRT and the CCRT systems show corresponding soot oxidation, however, in order to reduce the CO emissions the catalytic coating on the CDPF is essential, moreover the CCRT system shows remarkably higher $\text{HC}$ conversions than the CRT system. Hence CCRT system was found to be the definite most exploitable DPF system in this study.

From the investigation of $\text{NO}_2$ supported continuous regeneration it can be concluded that if the engine is running at approximately 50-60% engine load, with exhaust temperatures around 400$^\circ\text{C}$, it is possible to maintain a continuous regeneration of the DPF given that much of the $\text{NO}$ in the exhaust is oxidized to $\text{NO}_2$ upstream the DPF. The DPF soot mass equilibrium stage is dependent on the $\text{NO}_2$ concentration, thus lower engine back-pressure are at the expense of higher $\text{NO}_2$ emissions.

The possibility of triggering a $\text{O}_2$ based regeneration by idle gas conditions was also presented. This method can rapidly clean the DPF if a certain amount of soot is stored in the DPF ($>8\text{kgsoot}/\text{m}^3\text{DPF}$), and exhaust and DPF monolith temperatures are adequate (550$^\circ\text{C}$) when the idle conditions are initiated.

### 6.0.2 Simulation models and contributions

Requirements of aftertreatment technology on onboard diesel generators is being tightened, and possibilities and optimizations regarding retrofitting DPF systems in these auxiliary engines can be further investigated provided calibrated simulation models exists, such that strategies and conditions for successful DPF regeneration can be investigated while expensive and time consuming tests are avoided.

In the calibrated CDPF model it is possible to distinguish between thermal and catalytic soot oxidation, although the catalytic contribution to the soot oxidation is marginal. Also catalytic wall reactions are calibrated from the experimental data, which in combination with the catalytic soot oxidation presents the difference between the CDPF model and the NC DPF model. The thermal soot oxidation reactions are defined by an Arrhenius expression where the activation energies and pre-factors are calibrated to fit the experimental results, and with the identified parameters, which are...
equivalent for the CDPF and the NC DPF, the model presents soot burn rates well correlated with the experimentally measured rates. The identification of the activation energies and the frequency factors are important, as the same Arrhenius expressions can be applied in potential 3D models. The DPF pressure drop presented by the simulation models deviates somewhat from the experimental results. However, this difference only occurs at higher temperatures, during regeneration, and is concluded to be related to the physical nature of the soot oxidation.

With the current CDPF model a minimum monolith size for retrofitting a DPF in a larger engine can be determined from the maximum allowed engine back pressure. However, if the CDPF monolith have to be much larger than the tested CDPF the assumption of adiabatic temperature distribution might become invalid.

The soot oxidation in the DOC was accounted for in the model by deriving a temperature dependent expression for the outlet soot concentration relative to the measured inlet concentrations. Further calibration of the DOC model regarding soot oxidation requires more experimental data.

6.0.3 Future research

The aim of this thesis has been to investigate DPF system regeneration for the intention of removing the main part of the particulate matter from the exhaust from onboard diesel generators on large vessels. There was not enough time for defining simulations with conditions for an auxiliary engine, and investigating optimal DPF monolith size for such an engine, however, models are calibrated for such studies and several interesting observations has been made that can point out directions for further research.

A negative pressure drop gradient was measured for one of the CDPF tests although the DPF soot mass was increased. This occurred near initiation of the CDPF regeneration, and was believed to be caused by changes in the stored soot structure or distribution due to the soot oxidation. It would be interesting to investigate whether this phenomena is limited to the CDPF or if the NC DPF shows similar behavior, and in general to study the behavior of the soot oxidation in the different soot layers in DPFs.

The DOC showed surprisingly efficient soot oxidation, hence further testing in the area would be interesting, as well as necessary to calibrate a CAT model which also predicts the oxidation of soot in a DOC. Before a general model can be developed further measurements of the DOC soot burn rate is necessary to determine whether the soot oxidation presents consistency in the matter of exhibiting the approximate same rates at given temperatures. Further experiments could with benefits comprise studies of particulate sizes at the inlet and outlet of the DOC, such that an understanding of how the soot oxidation is occurring in the DOC can be studied.
From the comparison of the effect of the catalytical coatings on the CDPF and the DOC, optimizing the DOC performance with regards to $NO_2$ production should be in focus during optimization of DPF regeneration. Continuous $NO_2$-based regeneration was investigated, and if the temperature and $NO_2$ concentration is adequate, continuous regeneration of the DPF can be achieved. This requires a high $NO_2$ concentration which theoretically can be achieved with an upstream DOC. Characterizing real world DPF regeneration is difficult, but optimizing a reliable DPF system that can be regenerated continuously, without monitoring can be done with $NO_2$, and is an interesting subject for further studies.
Bibliography


[3] For information, see: Dinex AS, SiC - "silicon Carbide (SiC) diesel particulate filter (DPF)", at [http://www.dinex.dk].


Appendix A

A.1 BOOST model boundary conditions

In this section the measured exhaust properties and species concentrations necessary to generate simulation models for the CDPF and the DOC in BOOST are summarized.

The concentrations of $H_2O$ and $O_2$ are not measured, but have been calculated from the air-fuel ratio based on classical diesel cycle assumptions using Gaseq, a Windows 3.1 program for combustion equilibrium calculations. First adiabatic compression with compression ratio of 17.9 is assumed, and this is followed by isobar combustion, with adiabatic temperature and composition at the constant pressure calculated from the compression. The fuel hydrogen/carbon ratio is assumed to be 2, and air fuel ratio is calculated from the inverse air excess ratio, eq.(A.1). The computational methods for calculating lambda and the additional engine performance parameters are viewed in B.1.1.

The measured exhaust properties and species concentrations from the NC DPF tests are from ref. [11] and [12]. Table A.5 and A.6 presents the parameters used as BOOST model boundary conditions for the NC DPF simulations in 2010.

\[
\phi = \frac{1}{\lambda}
\]  

(A.1)

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A.1.1 BOOST model boundary conditions for the CDPF model

<table>
<thead>
<tr>
<th>Test no</th>
<th>Load [kpa]</th>
<th>[rpm]</th>
<th>[%]</th>
<th>$T_{in}$ [°C]</th>
<th>PM$_{c,in}$ [-]</th>
<th>G$_{exh,in}$ [kg/h]</th>
<th>P$_{DPF,out}$ [Pa]</th>
<th>$m_{soot,init}$ [kg/m$^3$]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>640</td>
<td>2500</td>
<td>37</td>
<td>305</td>
<td>0.2045e-4</td>
<td>177.5</td>
<td>106630</td>
<td>1.9076</td>
</tr>
<tr>
<td>2</td>
<td>768</td>
<td>2500</td>
<td>45</td>
<td>353</td>
<td>0.1999e-4</td>
<td>178.7</td>
<td>108790</td>
<td>3.5574</td>
</tr>
<tr>
<td>3</td>
<td>896</td>
<td>2500</td>
<td>52</td>
<td>383</td>
<td>0.1839e-4</td>
<td>186.1</td>
<td>109980</td>
<td>4.9753</td>
</tr>
<tr>
<td>4</td>
<td>1024</td>
<td>2500</td>
<td>60</td>
<td>411</td>
<td>0.2644e-4</td>
<td>175.6</td>
<td>113060</td>
<td>5.7486</td>
</tr>
<tr>
<td>5</td>
<td>960</td>
<td>3000</td>
<td>67</td>
<td>444</td>
<td>0.3214e-4</td>
<td>200.9</td>
<td>116730</td>
<td>6.0580</td>
</tr>
</tbody>
</table>

Table A.1: Gas properties for CDPF inlet boundary conditions

<table>
<thead>
<tr>
<th>Test no</th>
<th>λ</th>
<th>φ</th>
<th>CO$_2$ [%]</th>
<th>CO [ppm]</th>
<th>H$_2$O [%]</th>
<th>HC [ppm]</th>
<th>NO$_2$ [ppm]</th>
<th>NO [%]</th>
<th>O$_2$ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.311</td>
<td>0.434</td>
<td>6.42</td>
<td>165</td>
<td>5.86</td>
<td>19</td>
<td>117.9</td>
<td>625</td>
<td>11.3</td>
</tr>
<tr>
<td>2</td>
<td>2.041</td>
<td>0.455</td>
<td>7.29</td>
<td>161</td>
<td>6.13</td>
<td>18</td>
<td>131.2</td>
<td>766</td>
<td>10.8</td>
</tr>
<tr>
<td>3</td>
<td>1.798</td>
<td>0.560</td>
<td>8.31</td>
<td>134</td>
<td>7.45</td>
<td>20</td>
<td>204.5</td>
<td>1090</td>
<td>8.46</td>
</tr>
<tr>
<td>4</td>
<td>1.622</td>
<td>0.617</td>
<td>9.24</td>
<td>121</td>
<td>8.16</td>
<td>22</td>
<td>277.1</td>
<td>1545</td>
<td>7.22</td>
</tr>
<tr>
<td>5</td>
<td>1.660</td>
<td>0.603</td>
<td>9.02</td>
<td>134</td>
<td>7.99</td>
<td>27</td>
<td>253.7</td>
<td>1429</td>
<td>7.51</td>
</tr>
</tbody>
</table>

Table A.2: Species concentration at CDPF inlet

A.1.2 BOOST model boundary conditions for the DOC model

<table>
<thead>
<tr>
<th>Test no</th>
<th>Load [kpa]</th>
<th>[rpm]</th>
<th>[%]</th>
<th>$T_{in}$ [°C]</th>
<th>PM$_{c,in}$ [-]</th>
<th>G$_{exh,in}$ [kg/h]</th>
<th>P$_{DOC,out}$ [Pa]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>627</td>
<td>2500</td>
<td>37</td>
<td>313</td>
<td>0.2781e-4</td>
<td>159.0</td>
<td>109580</td>
</tr>
<tr>
<td>2</td>
<td>761</td>
<td>2500</td>
<td>44</td>
<td>364</td>
<td>0.1465e-4</td>
<td>163.6</td>
<td>108960</td>
</tr>
<tr>
<td>3</td>
<td>896</td>
<td>2500</td>
<td>52</td>
<td>399</td>
<td>0.1280e-4</td>
<td>167.9</td>
<td>111770</td>
</tr>
<tr>
<td>4</td>
<td>960</td>
<td>3000</td>
<td>67</td>
<td>465</td>
<td>0.3010e-4</td>
<td>199.1</td>
<td>117390</td>
</tr>
<tr>
<td>5</td>
<td>886</td>
<td>3500</td>
<td>72</td>
<td>496</td>
<td>0.6418e-4</td>
<td>239.0</td>
<td>122230</td>
</tr>
</tbody>
</table>

Table A.3: Gas properties for DOC inlet boundary conditions
A.1 BOOST model boundary conditions

<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2.308</td>
<td>0.433</td>
<td>6.42</td>
<td>171</td>
<td>5.86</td>
<td>21</td>
<td>112.6</td>
<td>657</td>
<td>11.27</td>
</tr>
<tr>
<td>2</td>
<td>2.016</td>
<td>0.496</td>
<td>7.38</td>
<td>147</td>
<td>6.66</td>
<td>18</td>
<td>127.6</td>
<td>807</td>
<td>9.87</td>
</tr>
<tr>
<td>3</td>
<td>1.771</td>
<td>0.565</td>
<td>8.44</td>
<td>139</td>
<td>7.52</td>
<td>21</td>
<td>237.0</td>
<td>1074</td>
<td>8.35</td>
</tr>
<tr>
<td>4</td>
<td>1.629</td>
<td>0.614</td>
<td>9.20</td>
<td>145</td>
<td>8.12</td>
<td>24</td>
<td>301.8</td>
<td>1464</td>
<td>7.28</td>
</tr>
<tr>
<td>5</td>
<td>1.680</td>
<td>0.595</td>
<td>8.90</td>
<td>176</td>
<td>7.90</td>
<td>28</td>
<td>228.8</td>
<td>1296</td>
<td>7.68</td>
</tr>
</tbody>
</table>

Table A.4: Species concentration at DOC inlet

A.1.3 BOOST model boundary conditions for simulating the NC DPF

Table A.5 and A.6 are from (Cordtz, 2010) [11].

<table>
<thead>
<tr>
<th>Test no</th>
<th>Load [kpa]</th>
<th>T_in [°C]</th>
<th>PM_c,in [μm]</th>
<th>G_exh,in [kg/h]</th>
<th>P_DPF,_out [Pa]</th>
<th>m_soot,init [kg/m³]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>542</td>
<td>2500</td>
<td>30</td>
<td>262</td>
<td>0.1640e-4</td>
<td>147.6</td>
</tr>
<tr>
<td>2</td>
<td>678</td>
<td>2500</td>
<td>37</td>
<td>298</td>
<td>0.1763e-4</td>
<td>154.2</td>
</tr>
<tr>
<td>3</td>
<td>384</td>
<td>2500</td>
<td>45</td>
<td>335</td>
<td>0.2550e-4</td>
<td>162.1</td>
</tr>
<tr>
<td>4</td>
<td>949</td>
<td>2500</td>
<td>52</td>
<td>371</td>
<td>0.3279e-4</td>
<td>162.5</td>
</tr>
<tr>
<td>5</td>
<td>1105</td>
<td>2500</td>
<td>61</td>
<td>403</td>
<td>0.3156e-4</td>
<td>163.6</td>
</tr>
<tr>
<td>6</td>
<td>1031</td>
<td>3000</td>
<td>68</td>
<td>437</td>
<td>0.4188e-4</td>
<td>200.5</td>
</tr>
<tr>
<td>7</td>
<td>949</td>
<td>3500</td>
<td>73</td>
<td>464</td>
<td>0.3881e-4</td>
<td>233.1</td>
</tr>
</tbody>
</table>

Table A.5: Gas properties for NC DPF inlet boundary conditions, Ref.[11]

<table>
<thead>
<tr>
<th>Test no</th>
<th>CO₂ [%]</th>
<th>CO [ppm]</th>
<th>H₂O [%]</th>
<th>HC [ppm]</th>
<th>NO₂ [ppm]</th>
<th>NO [ppm]</th>
<th>O₂ [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5.70</td>
<td>209</td>
<td>5.70</td>
<td>24</td>
<td>95</td>
<td>511</td>
<td>10.6</td>
</tr>
<tr>
<td>2</td>
<td>6.66</td>
<td>147</td>
<td>6.66</td>
<td>22</td>
<td>114</td>
<td>697</td>
<td>9.20</td>
</tr>
<tr>
<td>3</td>
<td>7.46</td>
<td>160</td>
<td>7.46</td>
<td>21</td>
<td>136</td>
<td>897</td>
<td>8.20</td>
</tr>
<tr>
<td>4</td>
<td>8.63</td>
<td>137</td>
<td>8.63</td>
<td>25</td>
<td>185</td>
<td>1147</td>
<td>6.50</td>
</tr>
<tr>
<td>5</td>
<td>9.78</td>
<td>132</td>
<td>9.78</td>
<td>22</td>
<td>271</td>
<td>1688</td>
<td>5.00</td>
</tr>
<tr>
<td>6</td>
<td>9.39</td>
<td>140</td>
<td>9.39</td>
<td>24</td>
<td>266</td>
<td>1527</td>
<td>5.40</td>
</tr>
<tr>
<td>7</td>
<td>9.14</td>
<td>146</td>
<td>9.14</td>
<td>24</td>
<td>298</td>
<td>1389</td>
<td>5.80</td>
</tr>
</tbody>
</table>

Table A.6: Species concentration at NC DPF inlet, Ref.[11]

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A.2 BOOST model frequency factors and activation temperatures

A.2.1 Frequency factors $E$ and activation temperatures $K$ for the DPF catalytic wall reaction

The frequency factors and activation temperatures for the oxidation reactions in the BOOST DPF catalytic wall reaction are tuned iteratively to fit the experimental results, and both the default values offered by BOOST and the applied values are shown for the HC, CO and NO oxidation in table A.7, A.8 and A.9 respectively.

<table>
<thead>
<tr>
<th>No</th>
<th>K $[kmol \cdot K/m^3 \cdot s]$</th>
<th>E $[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>8.2e9</td>
<td>6250</td>
</tr>
<tr>
<td>2</td>
<td>65.5 (default)</td>
<td>-921 (default)</td>
</tr>
<tr>
<td>3</td>
<td>2080 (default)</td>
<td>-361 (default)</td>
</tr>
<tr>
<td>4</td>
<td>3.98 (default)</td>
<td>-11611 (default)</td>
</tr>
<tr>
<td>5</td>
<td>479000 (default)</td>
<td>3733 (default)</td>
</tr>
</tbody>
</table>

Table A.7: Frequency factors and activation temperatures for oxidation of CO in the catalytic wall reaction

<table>
<thead>
<tr>
<th>No</th>
<th>K $[kmol \cdot K/m^3 \cdot s]$</th>
<th>E $[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.111e8</td>
<td>6000</td>
</tr>
<tr>
<td>2</td>
<td>65.5 (default)</td>
<td>-921 (default)</td>
</tr>
<tr>
<td>3</td>
<td>2080 (default)</td>
<td>-361 (default)</td>
</tr>
<tr>
<td>4</td>
<td>3.98 (default)</td>
<td>-11611 (default)</td>
</tr>
<tr>
<td>5</td>
<td>4.79e-8</td>
<td>3733 (default)</td>
</tr>
</tbody>
</table>

Table A.8: Frequency factors and activation temperatures for oxidation of HC in the catalytic wall reaction

<table>
<thead>
<tr>
<th>K</th>
<th>1.5e6</th>
<th>2.46e8</th>
<th>$[m^{1.5}/kmol^{0.5} \cdot s]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>E</td>
<td>51000</td>
<td>82000</td>
<td>$[J/mol]$</td>
</tr>
</tbody>
</table>

Table A.9: Frequency factor and activation energy for oxidation of NO
A.2 BOOST model frequency factors and activation temperatures

A.2.2 Frequency factors and activation temperatures for the DOC model

The frequency factors and activation temperatures for the BOOST DOC oxidation reactions are tuned iteratively to fit the experimental results, and both the default values offered by BOOST and the applied values are shown for the HC, CO and NO oxidation in table A.10, A.11 and A.12 respectively.

<table>
<thead>
<tr>
<th>No</th>
<th>K $[kmol \cdot K/m^3 \cdot s]$</th>
<th>E $[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.2e7</td>
<td>7100</td>
</tr>
<tr>
<td>2</td>
<td>65.5 (default)</td>
<td>-921 (default)</td>
</tr>
<tr>
<td>3</td>
<td>2080 (default)</td>
<td>-361 (default)</td>
</tr>
<tr>
<td>4</td>
<td>3.98 (default)</td>
<td>-11611 (default)</td>
</tr>
<tr>
<td>5</td>
<td>4.79e-8 (default)</td>
<td>3733 (default)</td>
</tr>
</tbody>
</table>

Table A.10: Frequency factors and activation temperatures for oxidation of CO

<table>
<thead>
<tr>
<th>No</th>
<th>K $[kmol \cdot K/m^3 \cdot s]$</th>
<th>E $[K]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>5500</td>
<td>4150</td>
</tr>
<tr>
<td>2</td>
<td>65.5 (default)</td>
<td>-921 (default)</td>
</tr>
<tr>
<td>3</td>
<td>2080 (default)</td>
<td>-361 (default)</td>
</tr>
<tr>
<td>4</td>
<td>3.98 (default)</td>
<td>-11611 (default)</td>
</tr>
<tr>
<td>5</td>
<td>4.79e-8 (default)</td>
<td>3733 (default)</td>
</tr>
</tbody>
</table>

Table A.11: Frequency factors and activation temperatures for oxidation of HC

<table>
<thead>
<tr>
<th>Default value Used in simulation, fig.5.19</th>
</tr>
</thead>
<tbody>
<tr>
<td>K</td>
</tr>
<tr>
<td>E</td>
</tr>
<tr>
<td>A</td>
</tr>
</tbody>
</table>

Table A.12: Frequency factor and activation energy for oxidation of NO
Appendix B

B.1 Computational methods

B.1.1 Engine performance parameters

The break power is estimated from the Eddy Current Brake as weight in kilo pounds (kp), and converted to power by the following formula:

\[ BP = \frac{0.7457 \cdot F \cdot N}{1000} \text{ [kW]} \] (B.1)

\[ \text{Break mean pressure} \]
\[ b_{mep} = \frac{120 \cdot BP}{V_d \cdot N} \text{ [Pa]} \] (B.2)

\[ \text{Engine total efficiency} \]
\[ \eta_t = \frac{BP}{\dot{m}_{fuel} \cdot H_u} \text{ [%]} \] (B.3)

\[ \text{Engine specific fuel consumption} \]
\[ spfc = 1000 \cdot \frac{G_{fuel}}{BP} \text{ [g/kWh]} \] (B.4)

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The \( \lambda \) value is calculated from the measured gas concentration by the following formula provided by ref.[1].

**Air Excess ratio**

\[
\lambda = \frac{\left(100 - \frac{CO \cdot 10^{-4}}{2} - HC \cdot 10^{-4}\right) + \left(0.45 \cdot \frac{1 - \frac{2 \cdot CO \cdot 10^{-4}}{CO + CO_2}}{1 + \frac{2 \cdot CO \cdot 10^{-4}}{CO + CO_2}}\right) \cdot (CO_2 + CO \cdot 10^{-4})}{6.9078 \cdot (CO_2 + CO \cdot 10^{-4} + HC \cdot 10^{-4})}
\] (B.5)

Where \( CO \) and \( CO_2 \) is the dry exhaust gas concentration of the two species in \( ppm \) and \( vol \% \) respectively, and \( HC \) is the concentration of \( HC \) in \( ppm \).

The formula was validated as a suitable calculation method in ref.[11].

**B.1.2 Particulate mass flow rate**

The computational method used to calculate the particulate mass flow rate of a soot sampling is given by ref.[1].

**Particulate Mass Flow Rate**

\[
M_{PT} = \frac{m_f}{M_{sam}} \cdot q \cdot \frac{G_{exh}}{1000} \quad [g/h]
\] (B.6)

Where the engine exhaust mass flow rate is calculated by using the excess air ratio \( \lambda \) and the measured fuel flow rate. For a Diesel fuel the stoichiometric air fuel ratio is set to 16.4.

**Engine exhaust mass flow rate**

\[
G_{exh} = G_{fuel} + G_{fuel} \cdot AF_r \cdot \lambda \quad [kg/h]
\] (B.7)

**Mass of diluted exhaust passed through the sample filter**

\[
M_{sam} = \frac{P_{amb} \cdot V_s \cdot M}{R \cdot T_s} \quad [kg]
\] (B.8)
B.1 Computational methods

Dilution ration

\[
q = \frac{CO_{2,\text{exh}} - CO_{2,\text{dilair}}}{CO_{2,\text{dilexh}} - CO_{2,\text{dilair}}} \quad [-] \quad (B.9)
\]

Dry-wet correction of raw exhaust gas

\[
CO_{2,\text{exh}} = k_{Wr} \cdot CO_{2,\text{exh}}
\]
\[
k_{Wr} = \left(1 - F_{FH} \cdot \frac{G_{\text{fuel}}}{G_{\text{air}}} \right) - k_{W2}
\]
\[
k_{W2} = \frac{1.608 \cdot H_a}{1000 + (1.608 \cdot H_a)}
\]
\[
F_{FH} = \frac{1.969}{1 + \frac{G_{\text{fuel}}}{G_{\text{air}}}}
\]
\[
H_a = \frac{6.22 \cdot R_{\text{amb}} \cdot p_a}{p_{\text{amb}} - (p_a \cdot R_{\text{amb}} \cdot 10^{-2})}
\]
\[
p_a = 10^{8.07131 - \frac{1730.63}{233.426 + T_{\text{amb}}}} \cdot \frac{101.325}{760}
\]

\[
CO_{2,\text{dilexh}} = k_{We2} \cdot CO_{2,\text{dilexh}}
\]
\[
k_{We2} = \frac{1 - k_{W1}}{1 + \frac{HCR \cdot CO_{2,\text{exh}}}{200}}
\]
\[
k_{W1} = \frac{1.068 \cdot H_d}{1000 + (1.608 \cdot H_d)}
\]
\[
H_d = \frac{6.22 \cdot R_d \cdot p_d}{p_{\text{amb}} - (p_d \cdot R_d \cdot 10^{-2})}
\]
\[
p_d = 10^{8.07131 - \frac{1730.63}{233.426 + T_{d}}} \cdot \frac{101.325}{760}
\]

Assumptions:

\[
T_d = T_{\text{amb}}
\]
\[
R_d = R_{\text{amb}}
\]

Dry-wet correction of dilution air

\[
CO_{2,\text{dilair}} = K_{Wd} \cdot CO_{2,\text{dilair}}
\]
\[
K_{Wd} = 1 - k_{W1}
\]
B.1.3 Average soot mass in DPF

Percent soot burn relative to average soot mass in DPF is calculated from the soot mass at the start of a test and the average DPF soot mass after an hour of steady state condition. Assuming steady state condition was reached after 20 min for all tests the test length considered is $t_{\text{mean}} = 80 \text{ min}$.

$$PT_{\text{stored}} = \frac{m_{\text{soot,end}} - m_{\text{soot,init}}}{\Delta t_{\text{test}}} \quad [g/h] \quad (B.10)$$

Where $m_{\text{soot,init}}$ and $m_{\text{soot,end}}$ are the measured soot mass before and after a test in [g], and $\Delta t_{\text{test}}$ is the actual measured time of each test.

$$PM_{\text{burned}} = PT_{\text{burned}} \cdot \frac{t_{\text{mean}}}{60} \quad [g] \quad (B.11)$$

Average soot mass in DPF

$$PM_{\text{stored,mean}} = m_{\text{soot,init}} + \frac{PT_{\text{stored}} \cdot 60}{t_{\text{mean}}} \quad [g] \quad (B.12)$$

The percent soot burn relative to average soot mass in DPF

$$\frac{PM_{\text{burned}}}{PM_{\text{stored,mean}}} \cdot 100 \quad [%] \quad (B.13)$$

B.1.4 Temperature correction

The model used for estimating the actual exhaust gas temperature at DPF/DOC inlet and outlet is provided by ref. [29], where it is stated that the thermocouple tip temperature can deviate from the actual gas temperature due to the following three factors: lumped thermal capacitance of the TC tip, conduction heat transfer between the TC tip and the pipe wall through the mounting holding the TC and radiation heat transfer between the TC and the surrounding pipe wall.
B.1 Computational methods

Energy balance

\[ \rho_c C_{TC} A_{TC} \frac{dT_{TC}}{dt} = \frac{d}{dx} \left( k_{TC} A_{TC} \frac{dT_{TC}}{dx} \right) \quad (B.14) \]

\[ -h P_{TC} (T_{TC} - T_{exh}) - \varepsilon \sigma P_{TC} (T_{TC}^4 - T_{wall}^4) \]

At steady state there TC temperature gradient \( \frac{dT_{TC}}{dx} \) is = 0, and heat conducted through the TC wire is neglected since the TC tip temperature gradient \( \frac{dT_{TC}}{dx} \) is ≈ 0. Thus the corrected gas temperature can be expressed by radiation, the third right hand term in eq. B.14, and the heat supplied to the TC, which is a convective heat transfer given by the second term.

Corrected exhaust gas temperature

\[ T_{exh,corr} = T_{TC} + \frac{\varepsilon \sigma}{h} (T_{TC}^4 - T_{wall}^4) \quad (B.15) \]

Where \( T_w \) is the measured pipe wall temperature, \( \sigma \) is the Stephan Boltzmann constant, \( \varepsilon \) is the emissivity, which assumed to be 1 due to internal black sooted surfaces and \( h \) is the heat transfer coefficient of the thermocouple. The heat transfer coefficient is coupled to the Nusselt number, which for a wire normal to the flow can be found from eq (B.16), according to ref. [31].

Nusselt number

\[ Nu = (0.44 \pm 0.06) \cdot Re^{0.5} = \frac{h d_{tc}}{k} \quad (B.16) \]

Where the properties of dry air is used to express the gas conditions. \( d_{tc} \) is the diameter of the TCs (\( d_{TC,1} = 1.1e - 3m \) and \( d_{TC,2} = 1.6e - 3m \)), \( k \) the thermal conductivity and \( Re \) the Reynolds number of the exhaust gas given by the TC diameter and the exhaust gas velocity.

Heat transfer coefficient of TC

\[ h = \frac{Nu \cdot k}{d_{tc}} \quad (B.17) \]

The pipe wall temperature was measured for the NC DPF, [11], and are seen in table ???. From the assumption of the wall temperature is equally lower for the CDPF as the NC DPF the following expression was formulated:

\[ T_{wall} = T_{TC} - 1.13 \cdot T_{room} \quad (B.18) \]
This expression was also applied for the DOC. For the CDPF which has the
same structure and isolation as the NC DPF the assumption is adequate,
while for the DOC there are higher uncertainties regarding the assumed wall
temperature.

<table>
<thead>
<tr>
<th>Test nr</th>
<th>1</th>
<th>2</th>
<th>3</th>
<th>4</th>
<th>5</th>
<th>6</th>
<th>7</th>
</tr>
</thead>
<tbody>
<tr>
<td>$T_{TC,NC,DPF}$ [°C]</td>
<td>260</td>
<td>295</td>
<td>329</td>
<td>350</td>
<td>374</td>
<td>410</td>
<td>454</td>
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<td>$T_{room,NC,DPF}$ [°C]</td>
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<td>32.5</td>
<td>35</td>
<td>37</td>
<td>39</td>
<td>41</td>
<td>45</td>
</tr>
<tr>
<td>$T_{wall,NC,DPF}$ [°C]</td>
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<td>257</td>
<td>287</td>
<td>308</td>
<td>330.5</td>
<td>366</td>
<td>411</td>
</tr>
</tbody>
</table>

**Table B.1:** Measured exhaust, room and wall temperatures for the NC DPF,
Ref.[11]