CZECH TECHNICAL UNIVERSITY IN PRAGUE FACULTY OF ELECTRICAL ENGINEERING



DIPLOMA THESIS

Modeling and Control of Aftertreatment Systems for Diesel Combustion Engines

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Modeling and Control of Aftertreatment Systems for Diesel Combustion Engines

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Název tématu: Modelování a řízení systémů pro redukci NOx a pevných částic dieselových spalovacích motorů

Pokyny pro vypracování:

 Seznamte se s problematikou redukce emisí dieselových spalovacích motorů.
 Vypracujte rešerši na téma systémů pro redukci škodlivých emisí používaných pro dieselové spalovací motory v automobilovém průmyslu.
 Na základě rešerše vyberte nejpoužívanější/nejrozšířenější systémy (SCR, DPF) a navrhněte jejich zjednodušené modely vhodné pro návrh řízení.
 Navrhněte vhodné řídicí strategie pro vybrané systémy. Navržené algoritmy ověřte pomocí simulací v Matlabu/Simulinku.

Seznam odborné literatury:

 [1] J.B. Heywood, Internal Combustion Engine Fundamentals, McGraw-Hill, 1988
 [2] L. Guzella, Ch.H. Onder, Introduction to Modelling and Control of Internal Combustion Engine Systems, Springer, 2004
 [3] Vybrané časopisecké publikace

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V Praze dne 15. 12. 2009

Declaration

I declare that I have created my Diploma Thesis on my own and I have used only literature cited in the included reference list.

In Prague, <u>10. 5. 2010</u>

it Do

signature

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Abstrakt

V této diplomové práci je představen model systému úpravy spalin dieselových motorů. Aktuální stav problematiky je pokryt podrobnou rešerší používaných technologií úpravy spalin, na jejímž základě je vybráno několik konfigurací systémů úpravy spalin. Porovnáním klíčových parametrů uvedených systémů byl vybrán k dalšímu studiu systém na bázi SCR jako nejvhodnější pro použití v sektoru těžkých nákladních automobilů.

Model systému úpravy spalin je implementován v programu MATLAB/Simulink a zahrnuje hlavní fyzikální a chemické procesy, které probíhají v obdobném reálném systému. Hlavní důraz při návrhu modelu je kladen na jednoduchost a přesnost tak, aby mohl být výsledný model použit pro účely simulace řízení a návrhu experimentů pro testování motorů. Model je validován sadou simulací, které zároveň objasňují vliv jednotlivých parametrů katalyzátoru na tvar statických převodních a dynamických přechodových charakteristik.

Pro získaný model je navržena řídicí strategie využívající data z modelu dieselového motoru, který byl poskytnut firmou Honeywell. Následně je na model systému úpravy spalin aplikována strategie řízení využívající jednoduchý PID regulátor. Ten umožňuje demonstrovat možnosti řízení získaného modelu systému úpravy spalin. Správnost modelu je ověřena sadou simulací, které zároveň objasňují vliv jednotlivých parametrů katalyzátorů na chování modelovaného systému.

Výsledky provedených simulací ukazují, že chování implementovaného modelu systému úpravy spalin poměrně přesně odpovídá předpokládanému chování obdobného reálného zařízení. Práce také ukazuje, že zpětnovazební řízení omezuje vliv poruch na chování systému úpravy spalin.

Abstract

A diesel exhaust gas aftertreatment system model is developed in this thesis. Based on detailed background research, an overview of current cutting edge exhaust gas aftertreatment technologies is presented. Acquired knowledge is exploited for the selection of several widely used aftertreatment system configurations. On the basis of major parameter comparison of presented system configurations, the SCR system is chosen for further study as the most suitable for heavy duty automotive application.

The aftertreatment system model is implemented in MATLAB/Simulink software and incorporates the major physical phenomena that take place in the comparable real device. The main emphasis of model development is placed on simplicity and relative accuracy, in order that the resulting model can be used for control simulation purposes and the design of experiments for engine testbed application. The model is validated through a set of simulations that also reveal the influence of particular catalyst parameters on model behavior.

A control strategy based on diesel engine model data provided by the Honeywell company is implemented. The obtained model is controlled by a simple PID controller, so that the possibilities of the aftertreatment system control can be demonstrated.

The results of conducted simulations proved that the developed model is sufficiently accurate. The conducted simulations and anticipated results are in line with expectations. Also it is shown in this thesis that the aftertreatment system feedback control strategy has a disturbance mitigation role.

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Nomenclature

Symbol	Meaning	Units
$A_{\rm cs}$	cross-sectional area of catalyst channel	$[m^2]$
$A_{\mathrm{f},s}$	frontal area of submodel s	$[m^2]$
$A_{\rm h,in}$	inner catalyst housing wall area	$[m^2]$
$A_{\rm h,out}$	outer catalyst housing wall area	$[m^2]$
A_k	pre exponencial factor of reaction rate \boldsymbol{k}	[1/s]
C_i	concentration of species i ,	$[mol/m^3]$
	denoted also as NO_{x} or NH_3 ect.	[ppm]
$C_{\mathrm{g},i}$	concentration of species i in gas phase	$[mol/m^3]$
$c_{\rm p,g}$	specific heat capacity of exhaust gas	$[J/(^{\circ}C kg)]$
$c_{\rm p,h}$	specific heat capacity of catalyst hous-	$[J/(^{\circ}C \text{ kg})]$
	ing	
$c_{\rm p,m}$	specific heat capacity of monolith	$[J/(^{\circ}C kg)]$
$C_{\mathrm{s},i}$	concentration of species i at surface	$[mol/m^3]$
$d_{\rm m}$	hydraulic diameter of catalyst channel	[m]
e	composite control error	
e_1	partial control error of NO_x	
e_2	partial control error of $\rm NH_{3,d}$	
$E_{\mathbf{a},k}$	activation energy for reaction k	$[J/mol^1]$
G_{a}	geometric surface area-to-volume ratio	[1/m]
$G_{\rm cat}$	active catalytic surface area	[1/m]
$h_{\mathrm{g} \to \mathrm{m}}$	convective heat transfer coefficient be-	$[W/m^2]$
	tween bulk gas and monolith	
i, j, k	indices	

IQ	injection quantity	[mg/stroke]
$k_{\mathrm{h}\rightarrow\mathrm{a}}$	heat conduction transfer coefficient be-	$[W/(m^2 \ ^\circ C^1)]$
	tween housing and ambient	
k_k	rate constant of reaction k	[1/s]
$k_{\mathrm{m} \rightarrow \mathrm{h}}$	heat conduction transfer coefficient be-	$[W/(m^2 \ ^\circ C^1)]$
	tween monolith and housing	
$k_{\mathrm{m},i}$	mass transfer coefficient of species i	[m/s]
$L_{\rm Pt}$	platinum adsorption site density	$[mol/m^2]$
M_i	molar mass of species i	[kg/mol]
\dot{m}_s	exhaust gas mass flow through sub-	[kg/s]
	model s	
$m_{ m h}$	mass of catalyst housing	[kg]
$N_{\rm eng}$	engine speed	[rpm]
$\mathrm{NH}_{3,\mathrm{d}}$	ammonia slip	[ppm]
n _{OC}	number of OC segments	
$n_{ m p}$	number of piping segments	
$n_{\rm SCR}$	number of SCR catalyst segments	
$Q_{\mathrm{h}\to\mathrm{a}}$	heat transferred from catalyst housing	[J]
	to ambient	
$Q_{\mathrm{m} \rightarrow \mathrm{h}}$	conductive heat transferred from mono-	[J]
	lith to housing	
R	universal gas constant	$[J/(^{\circ}C mol)]$
r_k	reaction rate of reaction k	[1/s]
$T_{\rm a}$	ambient environment temperature	$[^{\circ}C]$
$T_{\rm g}$	exhaust gas temperature	$[^{\circ}C]$
$T_{\rm g,in}$	inlet exhaust gas temperature	$[^{\circ}C]$
$T_{\rm g,out}$	outlet exhaust gas temperature	$[^{\circ}C]$
$T_{\rm h}$	catalyst housing temperature	$[^{\circ}C]$
$T_{\rm h,out}$	catalyst housing temperature in the	$[^{\circ}C]$
	outlet	
$T_{\rm m}$	monolith temperature	$[^{\circ}C]$
$T_{\rm m,out}$	catalyst monolith temperature in the	$[^{\circ}C]$
	outlet	
u	exhaust gas flow rate	[m/s]
$V_{\rm c}$	control volume	$[m^3]$

$V_{ m cat}$	volume of the whole catalyst	$[m^3]$
$V_{ m g}$	volume accessible for exhaust gas	$[m^3]$

Greek symbols

Δx	length of catalyst segment	[m]
$\Delta \mathrm{NO}_{\mathrm{x,ref}}$	NO_{x} reference	[ppm]
ε	void fraction	[1]
$arepsilon_{ m h}$	catalyst housing outer wall emissivity	[1]
η	NO_{x} reduction efficiency	[1]
$\theta_{ m NH3}$	ammonia surface coverage	[1]
ρ	NO_x control error gain	[1]
$ ho_{ m g}$	exhaust gas density	$[kg/m^3]$
$ ho_{ m h}$	catalyst housing density	$[kg/m^3]$
$ ho_{ m m}$	monolith density	$[kg/m^3]$
σ	Stephan-Boltzmann constant	$W/(m^2 \ ^\circ C^4)$
$\sigma_{i,k}$	stoichiometric coefficient of species i in	[1]
	reaction k	
φ	$\rm NH_{3,d}$ control error gain	[1]

Abbreviation

$\operatorname{CRT}^{(\overline{\mathbb{R}})}$	Continuous Regenerating Trap
CDPF	Catalysed Diesel Particulate Filter
DOC	Diesel Oxidation Catalyst
DPF	Diesel Particulate Filter
ECU	Engine Control Unit
EGR	Exhaust Gas Recirculation
ER	Eley-Rideal
FBC	Fuel-Borne Catalyst
FTP-75	Federal Test Procedure
HC	Hydrocarbon

IP	Intermediate Piping
LH	Langmuir-Hinshelwood
LNT	Lean $\mathrm{NO}_{\mathbf{x}}$ Trap
MPC	Model Predictive Control
NEDC	New European Driving Cycle
OC	Oxidation Catalyst
ODE	Ordinary Differential Equation
OP	Operating Point
PAH	Polyaromatic Hydrocarbon
PDE	Partial Differential Equation
pgm	platinum grade metal
PM	Particulate Matter
SCR	Selective Catalytic Reduction
SCR-Cat	Selective Catalytic Reduction Catalyst
SOF	Soluble Organic Fraction
TWC	Three Way Catalyst

Chapter 1

Introduction

Nowadays society increasingly realizes its non-negligible impact on the environment. Transportation is acknowledged as one of the major involved polluters. It is responsible for the emissions of nitrogen oxides (NO_x) , carbon monoxide (CO), hydrocarbons (HC) and particulate matter (PM). NO_x and PM have especially well documented negative effects on health and the environment [1]. Other pollutants are regulated as well, although these are not such an issue. As the public perceives the ecological and health concerns surrounding transportation, the authorities in most of the industrialized countries move towards increasingly stringent regulatory limits. The directives are divided into two main sectors due to the different technology of gasoline and diesel engines.

When it comes to the fuel efficiency issue and thus to carbon dioxide (CO_2) emissions, which are becoming a popular topic lately, the diesel engines attract the attention. State of the art diesel engines burn 35-50% less fuel than gasoline engines of comparable size [2]. Diesel engines are widely used to power the majority of buses, trucks and industrial equipment because of their superior fuel efficiency, durability and reliability.

Concerning passenger cars, consumers all over the world have noticeably shifted their preferences towards diesel propulsion. This behavior is mostly apparent in Europe, where diesel powered passenger cars are accounting for roughly 50% of the new sale car market. But unlike in Europe, in the USA diesel cars are holding a relatively small market share. It is likely that the more fuel prices rise, the more the consumers will move from gasoline to diesel propulsion in the USA. Car manufacturers are aware of this upcoming trend. But only emission-compliant cars can be introduced to the market. That is the main reason why emission abatement is gaining such importance.

Geographical focus of regulatory development has been in the European Union (EU). The first Euro I regulation came in the early 90's. It was followed by gradually tightening

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regulations until Euro III. Car manufacturers coped with those regulations by increasing injection pressure for lower PM and by introducing retarded injection for lower NO_x emissions [3]. Further emission limits introduced in Euro IV could not be achieved by engine measures alone. As a solution several car manufacturers opted for Exhaust Gas Recirculation to lower combustion temperature and thus lower NO_x emissions. Others applied Selective Catalytic Reduction technology with a water-urea solution as a reagent. Euro V was achieved by increased efficiency of contemporary exhaust gas aftertreatment systems. Impending Euro VI will bring in, as shown in Figure 1.1, even more stringent emission limits for light and heavy duty engines marketed in Europe.



Figure 1.1: Historical view of EU emission standards for diesel engines

A similar situation concerning emission regulations occurred in the USA, where legislation called Tier 1 and Tier 2 [4] was adopted for light-duty on-road vehicles. A progressive stringency of eight permanent certification levels called 'certification bins', that were fully introduced in 2009 as a part of Tier 2 legislation, is depicted in Figure 1.2. Beyond that a further tightening of emission limits in the USA is on the way.

Continuing development of aftertreatment systems is necessary to comply with upcoming European and American regulatory limits. The need for cleaner diesel engines is driving development, but the fuel efficiency of current diesel engines remains the same or even slightly lower in comparison with diesel engines from decade ago [3]. Thus, new developments in diesel engines will likely improve both emissions output as well as fuel consumption. It is obvious that without accurate models of aftertreatment systems and advanced control strategies it will be far more challenging for car manufacturers to develop future emission-compliant engines.



Figure 1.2: Tier 2 emission standards for passenger cars in USA

1.1 Objectives of the Thesis

The primary objective of this thesis is to propose a EURO VI-compliant exhaust gas aftertreatment system that will consider the needs of heavy duty automotive applications. Based on preliminary background research, a mathematical model of the selected exhaust gas aftertreatment system has to be developed and implemented in MATLAB/Simulink. The model is intended to be used for engine testbed calibration and for control as a subsystem of a complex engine model. Such a model will have to be relatively accurate and also sufficiently simple in order to allow fast deployment and calibration for control purposes.

The secondary objective is to propose, develop and implement a suitable control strategy for an exhaust gas aftertreatment system in MATLAB/Simulink. Furthermore, the validity of the implemented control strategy and of the aftertreatment system model will have to be verified by appropriate simulations.

1.2 Methods

The objectives of this thesis are accomplished via mathematical modeling based on information gained from detailed background study of the topic. A mathematical model of a diesel exhaust gas aftertreatment system will be implemented in MATLAB/Simulink while utilizing Level 2 M-file S-functions¹. Rather a simple control strategy will be applied, because of the work will be focused primarily on an aftertreatment system model development.

1.3 Outline of the Thesis

- Chapter 1 Introduction presents the studied topic and proposed goals of the thesis. It gives insight to the NO_x legislation and points out the importance of the exhaust gas aftertreatment systems.
- Chapter 2 Overview of Emission Reduction Technologies contains a detailed overview of currently used technologies for emission mitigation with emphasis on catalytic and filtration technologies.
- Chapter 3 Consideration of Aftertreatment System Concepts describes selection of the aftertreatment technology, while keeping in mind particular vehicle needs. Selected aftertreatment technology is further used for model development and control.
- Chapter 4 Complete SCR System Model introduces SCR model developed according to the cutting edge knowledge in the literature. The main governing phenomena and underlying reaction mechanism are described in detail.
- Chapter 5 Validation of the Aftertreatment System Model presents testing of developed submodels. Also an influence of catalyst parameters on catalyst behavior is studied thoroughly.
- Chapter 6 SCR System Control presents simple demonstration control strategy for developed SCR system model. The control strategy is tested on realistic diesel engine model data provided by Honeywell company.
- Chapter 7 DPF Model briefly views possibilities for DPF modeling.
- Chapter 8 Conclusion summarizes goals and obtained results of the thesis.

¹'The Level-2 M-file S-function allows user to create custom blocks with multiple input and output ports capable of handling any type of signal produced by a Simulink while utilizing MATLAB M language.' Paraphrased from MATLAB Help.

Chapter 2

Overview of Emission Reduction Technologies

The market, regulatory bodies and the desire of fuel economy are making great demands on diesel engine technology. The tailpipe emission output is considered one of the key areas of interest both for governments and car manufacturers. Hence the emitted exhaust is subject to strict regulation. Although the regulated emissions contain various types of polluting chemical compounds, the most watched are NO_x and PM emissions. To lower both mentioned main pollutants car makers have developed several efficient de NO_x and exhaust gas aftertreatment technologies during past 40 years. The most relevant and promising technologies for NO_x and PM emission abatement, as noted in background research, appendix ?? on page ??, will be described in this chapter.

2.1 NO_x Reduction Technologies

Since the diesel engine does not contain direct ignition, unlike a gasoline engine, it operates with higher in-cylinder compression pressure. This causes higher combustion temperature and it consequently leads to extensive NO_x formation. Two distinct approaches on how to avoid undesirable NO_x tailpipe emissions exist. The first approach, denoted as Exhaust Gas Recirculation (EGR), favors preventing NO_x formation by lowering the peak combustion temperature. The other approach relies on catalytic reduction of NO_x present in exhaust gases. The most promising catalytic technologies capable of sufficient NO_x reduction are the Selective Catalytic Reduction (SCR) and the Lean NO_x Trap

2.1.1 Exhaust Gas Recirculation

The EGR is a NO_x abatement technology used mostly in US heavy-trucking diesel applications. Since the EGR prevents NO_x formation, it does not need any additional reducing agent unlike the SCR.

The principle of this technology is shown in Figure 2.1. A portion of exhaust gas is diverted from the exhaust manifold into piping connected to the EGR cooler, where hot exhaust gas is substantially cooled. The cooling allows greater mass of recirculated exhaust gas to be introduced through EGR piping to the intake manifold and subsequently into the engine cylinder. Since exhaust gas contains substantial quantities of CO_2 and water vapor, it has also higher specific heat in comparison with air. Recirculated gas therefore dilutes air/fuel charge and thus lowers peak combustion temperatures. The amount of recirculated exhaust gas can be precisely controlled by the EGR Control valve.



Figure 2.1: Schematic of diesel engine with EGR system

However there are also shortcomings related with EGR usage. The EGR decreases the specific heat ratio of the combustion gases in the power stroke and therefore it reduces the reachable amount of power that can be utilized by the piston. The EGR also reduces the amount of burned fuel in the combustion cycle, thus the power output of the engine is lower than it could be without EGR utilization. The remaining unburned fuel (mostly carbon) tends to cause excessive PM formation. Consequently the PM has to be removed by other measures such as particulate filters, which will be discussed later in subsection 2.2.1.

Several distinct configurations of EGR exist in the literature [5]. With exception of the internal EGR, the other setups require substantial adjustments of engine design to fit a complete emission abatement system. Thus implementation of EGR is relatively expensive as it is shown in [6]. Herewith, an EGR equipped vehicle is more expensive and less competitive than a vehicle without EGR.

Pros:

- Mitigate NO_x without need of an additional reagent
- Saves weight unlike system with urea solution tank

Cons:

- Excessive PM formation
- Reduced fuel efficiency
- Expensive engine design adjustment

2.1.2 Selective Catalytic Reduction

The SRC is emerging as a one of the key NO_x abatement technologies in both the lightduty and heavy-duty automotive sectors. It has been around since the 1970's for stationary applications [7], e.g. for fossil fired power plants, where it showed excellent performance. The first commercially feasible urea-SCR systems for European and Japanese automotive heavy-duty automotive applications were introduced in 2004. Unlike conventional Three Way Catalysts (TWC) for gasoline engines, the diesel catalytic converters work under different conditions due to an excess of oxygen in the exhaust gas. Therefore an additional reducing agent is necessary. Suitable for this purpose could be the ammonia (NH₃) due to its good selectivity towards NO_x , except when transportation of pure ammonia is not desired nor advisable. In this case, the urea is used as an inoffensive non-poisonous reducing agent in automotive applications instead.

A simplified SRC system schematic is depicted in Figure 2.2. The injection of ureawater solution, available as AdBlue, to the piping upstream the SRC catalyst is controlled by a dosing unit. After injection, urea is thermally hydrolyzed to form ammonia and CO_2 . Afterwards, the released ammonia is stored in a catalyst porous washcoat surface, where it subsequently reacts with nitrogen dioxide (NO₂). The product of that reaction is water vapor and diatomic nitrogen. The complete reaction mechanism is described later in chapter 4.



Figure 2.2: Schematic of SCR system

Unfortunately, the transient unsteady operating conditions of diesel engine prevent to reach full 100% reduction of NO_x . This especially refers to the varying exhaust gas temperature, since the effective temperature window of the SCR is from 200 °C to about 450 °C. The NO_x reduction capability of the catalytic converter is significantly decreased outside this temperature window. This is caused by incomplete urea hydrolysis and low reaction rate, which results in a poor NO_x reduction efficiency mainly under low temperature conditions as well as in prevailing NH_3 desorption and subsequent conversion directly to nitrogen under high temperature conditions. To partially avoid a lack of low temperature efficiency, the current state of the art SRC catalysts incorporate the function of a urea hydrolyzing catalyst, therefore the use of an additional urea-hydrolyzing catalyst is not necessary [8]. A supplementary solution includes an additional heating to improve reaction rates during low temperatures. Further improvements in catalyst structure and function will be required since low temperature conditions are dominat during the European (NEDC) as well as US (FTP-75) test cycles [9]. When optimal temperature conditions are satisfied the NO_x reduction efficiency of SCR technology could be as high as 95% [10].

When heated, the SCR catalyst can store significant amount of NH_3 . The ammonia storage capacity declines with descending temperatures. Serious problems arise when the temperature of the exhaust gas suddenly drops. Part of accumulated NH_3 , proportional to the temperature drop, is released and NH_3 slip is likely to occur. Ammonia slip, i.e. ammonia presence in the SCR catalyst downstream, is closely watched by regulations, because of ammonia's distinctive odor and overall toxicity. Ammonia slip can be controlled by inclusion of an ammonia slip catalyst downstream the SCR catalyst or by application of advanced control strategies of urea injection.

Common automotive catalysts (applies to both SRC and LNT technologies) have a structure as shown in Figure 2.3. Catalysts consist generally of a ceramic monolith that is held by an intumescent mat, end seals to prevent gas leakage, a stainless steel can to house the monolith and mat, flanges to mount the catalyst to the exhaust piping, and a heat shield to protect adjacent components, the floor pan and ground vegetation from excessive thermal radiation [11].



Figure 2.3: Structure of common catalytic converter package [11]

A robust converter package provides positive holding pressure on the ceramic monolith substrate. It allows exhaust gas to enter the monolith evenly and serves as thermal insulation for the monolith. Thus it permits rapid heating of the monolith along with retention of the exothermic heat needed for catalytic reactions while minimizing radial temperature gradient. The package also provides an adequate hold on the mat and monolith to resist the vibrational and backpressure loads that would otherwise result in slippage of the monolith inside the can [11].

The ceramic monolith substrate, a key component of the SRC catalytic converter, can be fabricated by two distinct approaches [12]. The first approach is to use a single full catalyst that has a wall made of catalytic material. The second approach is to use a coated metallic or cordierite inert substrate. These substrates carry less active catalytic material and thus possess less low-temperature performance than of full catalysts. However, the low temperature performance can be somewhat enhanced by increasing the ratio between NO and NO₂ to about 50/50 over a base metal type Oxidation catalyst placed upstream the main SRC catalyst. The efficiency improvement of an SRC system enhanced with an oxidization catalyst could be around 30% [12].

The honeycomb ceramic monolith, shown in Figure 2.4, is widely used because of its particular properties such as a high surface area and a low pressure drop. Desirable properties of the monolith can be further improved by application of a so-called washcoat. According to the [3], the most common washcoat is titanium dioxide (TiO₂). Washcoat itself is a porous material, and when coated onto a support substrate it further increases the surface area and thus potentially increases the reduction capability of the catalyst. The washcoat is covered with catalytically active elements, mostly platinum grade metals (pgms) such as Pt, Pd or Rh. The amount of pgm used significantly affects both NO_x reduction efficiency and the price of the catalyst.

The SCR technology has difficulty concerning urea packing issues. Although the SCR technology offers great NO_x reduction potential for a reasonable price [6], many car owners prefer other $DeNO_x$ technologies because of the need to refill urea along with refueling. This is apparent in the US heavy trucking applications because of a relatively large and heavy urea tank. Consumption of urea varies from 1 to 7% [6] of total fuel consumption according to the used technology and control strategy. The urea packaging problem would be even more apparent if the SRC technology would be used for light-duty applications. The recent effort by Chrysler proposes that enough urea be kept onboard of the vehicle to allow refilling during lubrication oil changes [10]. This measure would mitigate the apparent disadvantage of SCR technology and allow the SCR usage even in

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passenger cars.



Figure 2.4: Structure of ceramic monolith and washcoat, based on [3]

Pros:

- $\bullet\,$ High $\mathrm{NO_x}$ reduction potential, widely anticipated to be around 95% [10]
- Wide operation temperature window 200-400 °C
- Successful stationary applications experience
- Government support of distribution infrastructure

Cons:

- The packaging issues related to supplementary urea tank
- $\bullet\,$ High possibility of $\rm NH_3$ slip occurrence (can be solved by $\rm NH_3$ slip catalyst)
- Low temperature performance

2.1.3 Lean NO_x Trap

The LNT or NO_x adsorber catalyst is a discontinuously operating aftertreatment technology [9]. LNT has three operating phases, as seen in Figure 2.5, that are repeated periodically. The first operation phase entails the reaction of NO_2 with a basic adsorbent (alkaline earth oxide, e.g. BaO) to form a nitrate or a nitro-compound under lean conditions. Since approximately 90 % of NO_x engine output is released in the form of NO, the NO has to be oxidised to NO_2 over a platinum-based catalyst first [2].

When the maximum capacity of LNT is reached, the second operation phase, NO_x trap regeneration, occurs. The adsorbed NO_2 is released and ultimately reduced to N_2 during rich conditions. The rich conditions are established by injection of the proper amount of hydro-carbon (HC) (e.g. diesel fuel) as a reducing agent. The effective operating temperature range of the adsorber is 300 °C to 400 °C [2]. The end of the storage and reduction phases are either indirectly calculated using models together with a Lambda Oxygen Sensor signal or more directly switched with an NO_x -sensor downstream the catalytic converter [8]. The NO_x storage phase lasts 60 s and the regeneration phase lasts 5 s [13], resulting in 8.3% decrease of average NO_x reduction efficiency¹



Figure 2.5: Operation phases of LNT catalyst [9]

¹Not accounting duration of the LNT desulphurization phase

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The last operating phase is closely related to the catalyst aging and deactivation by sulphur oxides (SO_x) that originate from sulphur contained in fuel and lube oil. Adsorption of SO_x on the NO_x adsorption sites deteriorates the NO_x reduction capability of LNT. That is an issue even with usage of low-sulphur fuels. During the last operating phase of LNT the desulphurization takes place under rich conditions and at temperatures exceeding 700 °C. Such a high temperature is achieved by introducing fuel to the catalyst via injection to the exhaust piping or via engine measures, e.g. late injection, while the exhaust valve is still opened. Sulphur poisoning can be reduced also by usage of a desulphurization catalyst upstream the LNT. But herewith the complexity of aftertreatment systems grows significantly.

Controlling the temperature of the desulphurization process within the 700 °C to 800 °C range is very challenging. High temperature can easily cause meltdown of catalytic material especially under an excess of oxygen. The catalytic material can later recrystallize randomly across the catalyst monolith resulting in a permanent drop of LNT performance [5]. Therefore removal of excess oxygen is crucial for the regeneration of the NO_x adsorber. To avoid severe thermal aging, sophisticated control strategies and engine optimization methods that will reduce the quantity of excess oxygen during regeneration have to be developed. Thermal aging is also connected with substantial loss of capacity over time. According to the [10], earlier LNTs lost perhaps 50% of their capacity over 15 to 20 desulphurisation cycles. Although newer versions now lose only about 25% of the capacity, additional improvement will be necessary to produce more durable LNTs.

During desulphurization most of the sulphur goes away in form of hydrogen sulphide (H_2S) which is highly poisonous and can not be released directly into the atmosphere. Hence an additional H_2S Oxidation catalyst downstream the LNT is likely to be used.

The LNT catalytic converter has a common catalytic structure, as seen earlier in Figure 2.3. Since the LNT technology requires the catalyst volume to be several times larger than cylinder capacity [5], it is not likely to be used for heavy-duty applications. This potential restriction appears to be not so problematic for usage in light-duty applications because of lower cylinder swept volume. Therefore LNT will likely be used mainly for light-duty applications.

When all conditions are satisfied, the LNT technology offers high NO_x reduction efficiency. Steady-state engine experiments with low-sulphur fuel have shown an NO_x reduction efficiency of almost 95% [2]. If the effects of catalyst aging and sulphur poisoning will be taken into account, an anticipated 60% to 70% of 'real-world' NO_x reduction efficiency for light-duty systems [10] can be reached. Therefore if a subsequent NO_x abatement technology will be used along an LNT, it is supposed that this will suffice for production of future emission compliant engines.

Pros:

- $\bullet\,$ High $\mathrm{NO_x}$ conversion efficiency: around 60-70% when aging accounted
- DeNO_x regeneration by engine internal measures
- The diesel fuel can be used as a reducing agent
- Unlike urea-SCR no distribution infrastructure needed

Cons:

- Rapid sulphur poisoning from fuel and lube oil [2]
- Difficult to control desulphurization process
- Fuel penalty due to the need for fuel injection during rich regeneration phase
- Increased complexity of the combined $DeNO_x$ and $DeSO_x$ aftertreatment system

2.2 PM Abatement Technologies

The soot or PM, more generally, is emitted by all kind of incomplete combustion of diesel fuel in diesel engines. It consists of carbon, inorganic oxides, and hydrocarbons, including some highly toxic polyaromatic hydrocarbons (PAHs) [14]. Most PM particles are sized 5-20 nm. Current legislation applies to all particulate matter that could be filtered and measured. Due to continuing research and discussions about the impact of nanoparticles on health, there will be changes in the legislation in the future. The size and number of particles will probably be regulated once suitable measurement technologies are available.

PM emissions can be reduced by better combustion, i.e. higher combustion temperatures with excess of oxygen, in the engine [14]. Unfortunately, these conditions will result in an increase in NO_x emissions, that are, like PM emissions, also strictly regulated. Involved phenomena is often denoted as PM/NO_x trade-off and is connected mostly with the function of the EGR [10]. Therefore, complying limits of PM pollution must be achieved otherwise. The most common solution to abate PM emissions is the Diesel Particulate Filter (DPF) and its variations like the Catalysed DPF (CDPF) and the Continuous Regenerating Trap (CRT[®]). Recently a Diesel Oxidation Catalyst (DOC) emerged as an additional PM reduction solution. Both mentioned counter-PM technologies and their modifications will be presented in this section.

2.2.1 Diesel Particulate Filter

The DPF is a flow-through device, that captures and accumulates particulate matter/soot in a trap. When the trap is full, i.e. it is loaded with certain amount of soot, the soot has to be removed through a regeneration process. Otherwise the soot will block the filter resulting in a rise of backpressure and consequently in a severe performance degradation of the engine. The filter regeneration process has to be introduced periodically by thermal means. Soot starts to burn-off spontaneously if the temperature reaches about 600 °C. The soot ignition temperature threshold can be lowered to approximately 300-400 °C by active catalytic species (Fe, Cu, or Ce) [14], [15] presence in the inner filter coating or in form of fuel additives. First mentioned applies for the Continuous Regenerating Trap (CRT[®]) and for the Catalysed DPF (CDPF), the second applies for the Fuel-Borne Catalyst (FBC) [10]. For the mentioned cases a passive regeneration process takes place. Nevertheless, the passive filter regeneration is not robust and is susceptible to cold climates, for such even the decreased soot ignition temperature is still not low enough to be reached in an exhaust gas system of light to medium duty applications, e.g. city buses and stop-and-go urban traffic. Therefore, an additional heating instrument is necessary to control the active regeneration process of the filter. Possible heating means include a fuel burner [5], electric heater or microwave heater [2] to obtain a temperature high enough for soot ignition. Both approaches increase the complexity of the filtering device. Alternatively, diesel fuel can be introduced to the filter by motor means, e.g. late fuel injection. According to the literature, the conventional particulate filters that have been catalyzed have exhibited 85 to 95% PM filtration efficiency [2].

The overloading of the filter with soot is an important issue. An overload of only 3-4 grams per liter of filter volume causes a rise in regeneration temperature in the order of 300-400 °C. The filter has to withstand conditions during the thermal regeneration process. Local rise of the temperature depends on properties of the filter material (thermal capacity and conductivity) as well as exhaust mass flow and temperature [14]. The worst case scenario is to stop the engine when the soot burn-up is taking place in a fully loaded trap. The temperature can rise locally to over 1300 °C, which can be high enough to

cause meltdown of the ceramic monolith body and even to ignite a vehicle. Therefore, reliable regeneration control technologies will be crucial to achieve satisfactory durability and long in-service life of the DPF. Possible solutions will likely include a DFP state space model or a special integrated design of the DPF [16].

The filter regeneration process could provide some synergies with the $DeNO_x$ system. This issue is connected with soot burn-up, which depends mainly on the oxygen and NO_x portion in exhaust gas. As well as O_2 , the NO_x can be used for soot oxidization thus effectively reducing the amount in exhaust gas needed for further removal. Furthermore the heat released from the exothermic reaction could improve efficiency of the downstream $DeNO_x$ system.

After soot burn-off, only incombustible substances remain in the filter. Their sources are mainly lubricating oil, fuel additives, salts from ambient air and motor wear and they consist mostly of oxides, sulfates and phosphates of iron, calcium and zinc. Usage of FBC also contributes to the total amount of incombustible remains. The ash accumulation in the filter leads to backpressure increase and to the decline of filtering capacity [14]. Therefore it effectively limits useful life of the filter. Increased deterioration of the filter is also caused by the chemical interaction of accumulated ashes with the material of the filter during high temperature regeneration cycles.

There are many different technologies of fabrication of particulate filters for automotive applications. They can be divided into following categories: ceramic wall flow, ceramic fiber, ceramic foam, electrostatic, metal non blocking and sintered filters [17]. Currently, the most often used filter fabrication technology is ceramic wall flow due to its high filtration efficiency, mastered production and cost. Several common materials for DPF monolith fabrication and their basic properties are given in table 2.1.

Ceramic monolith, which has a high amount of parallel channels, is a commonly used DPF structure. Such a monolith is very similar to the ceramic honeycomb monolith of the

Material	Cordierite	\mathbf{SiC}	\mathbf{SiN}	Mullite
$\overline{\text{Density } (g/cm^3)}$	2.1	3.1-3.2	3.2-3.4	2.9
Thermal conductivity (W/mK)	1-3	90	30	4-5
Thermal expansion $(10^{-6} \text{ cm}/^{\circ}\text{C})$	1	5	3.7	4
Young's modulus (Gpa)	130	410	310	150
Maximum operating temp. (°C)	1200-1400	1550-1650	1200-1540	1450

Table 2.1: Properties of selected DPF monolith materials [14], [11]

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previously mentioned DeNO_x catalysts, as seen in 2.1.2. Figure 2.6 shows a filter section with the exposed ceramic monolith, the wall-flow filtering principle and the regeneration cycle. Every channel of the monolith is alternatively closed on either the front or back side. Therefore exhaust gas is forced to flow through the porous walls (the so-called wall-flow-filter). Carried particulate matter is afterward deposited in wall pores. On the exit side of the filter the purified exhaust gas flows away. Generally used ceramic monoliths have square shaped channels with a density of about 200-300 cells per square inch (cpsi) and a wall thickness of about 350-400 μ m [17]. Special cases exist, where alternative channel shape is used to increase ash storage capacity [17].



Figure 2.6: Principle of the DPF [18]

Pros:

- High PM filtration efficiency: up to 95%
- Well mastered fabrication technology
- \bullet Could provide synergies with $\mathrm{DeNO}_{\mathrm{x}}$ system

Cons:

- Difficult to control regeneration process
- Exothermic heat safety issues
- Fuel penalty when using fuel burner

2.2.2 Diesel Oxidation Catalyst

The DOC is a flow-through device that consists of a stainless steel canister containing a honeycomb monolith structure coated with an active catalytic layer of pgm. Thus it is having the same structure as the $DeNO_x$ catalysts, see Figure 2.3.

The DOC is used for a minor reduction of unwanted emissions from diesel exhaust. The exhaust gases flowing through the DOC contain CO, gaseous and liquid phase HC and soluble organic fraction (SOF). These substances are oxidized in the DOC and therefore the total amount of undesirable pollutants is decreased. The DOC exhibits around 80-90% removal efficiency of SOF and CO under optimal conditions. Also the reduction of PM is becoming an important function of modern DOC. About 30% of the total PM mass of diesel exhaust is attributed to liquid HC, or SOF according to the [19]. Therefore if the main fraction of SOF is removed, the total PM conversion efficiency can be usually a little over 20%. Conversion efficiences of the DOC are highly dependent on the influence of actual application, device age and condition, exhaust gas composition and actual suplhur levels.

The oxidization of CO and HC takes place under certain temperature conditions. Ambient temperature is not satisfactory for the oxidization reaction to occur. However the DOC greatly benefits from its smaller volume in comparison with a normal DPF or with other catalysts. Thus the DOC is heated up by hot exhaust almost immediately after the engine has started, so both oxidization reactions take place more quickly [20]. The lowest temperature for which oxidation reaction occurs is often denoted as a light-off. After reaching this specific temperature, reduction efficiencies rise quickly to the steady state values.

Although the DOC does not suffer rapidly from the sulphur concentrations, the PM reduction efficiency of the device can be improved when low-sulphur fuels are used. As well as the DFP, the DOC is vulnerable to thermal degradation if it is exposed to high temperatures above 650 °C for long periods of time. The DOC can be poisoned by certain chemical elements such as phosphorus lead and heavy metals [19]. Some of these substances are contained in engine lube oil. Therefore usage of low-phosphorous lube oils along with low oil consumption can prevent the catalyst damage.

A special type of DOC² is commonly used in combination with the SCR catalyst. It is placed upstream the SCR since it used for oxidization of NO to NO₂. Such a catalyst alters the NO₂/NO ratio to about 50/50, which is favorable for the increase in the overall

²Denoted as Oxidation Catalyst (OC).
NO_x reduction efficiency of the SCR catalyst. Moreover heat released from CO as well as from oxidation of unburned diesel fuel remains in exhaust gas can serve as auxiliary heating to the SCR catalyst and thus it can improve the NO_x reduction behavior of the SCR catalyst under low temperature conditions.

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In addition to abating the harmful content of the exhaust, the DOC can be used as an auxiliary means for introduction of the DPF regeneration, provided that the DOC is placed upstream the DPF. The DOC ensures combustion of the injected diesel fuel and thus it produces a temperature high enough to ignite the regeneration process in the soot filter. In this case it is not necessary for the DOC to be placed close to the engine since the HC can be introduced via special injection system, which can be located in front on the DOC. However such usage of the DOC naturally results in increased fuel consumption.

Technology of catalytic filters is undergoing rapid progress. Recent reports show that costly pgm loading can be reduced and the performance increased if the DOC function is incorporated into the particulate filter via new coating methods [10]. Then loaded soot can be burned more completely in comparison with filtering systems with separate DOC or FBC [21].

Pros:

- Additional PM reduction efficiency: up to 20%
- Reduces amount of HC, SOF and CO in exhaust gas
- Synergy with both downstream placed DPF or SCR

Cons:

- Adds complexity to exhaust gas aftertreatment system
- Suffers from thermal degradation
- Possible poisoning by lead and phosphorus from lube oil
- Adds fuel penalty if used as a auxiliary DPF regeneration introduction mean

Chapter 3

Consideration of Aftertreatment System Concepts

In this chapter, various aftertreatment system concepts are compared. Based on a conducted comparison, an appropriate aftertreatment system configuration is chosen for further model development effort.

3.1 Overview of Aftertreatment System Setups

To meet tightening emission limits of PM and NO_x , car manufacturers have to consider usage of a NO_x aftertreatment system in combination with a DPF. Two distinct DPF placement options exists. The DPF can be placed upstream or downstream of the NO_x aftertreatment unit. Another relevant part of the aftertreatment system to be considered is a DOC. If the DOC is placed upstream of the $deNO_x$ device¹ as well as upstream of the DPF, it further improves emission reduction capabilities of the stated aftertreatment devices. Unlike urea-based SCR catalyst systems, the LNT provides the potential to be placed in a close-coupled location to the engine and/or to be split into two separate bricks, as it is suggested in [9].

Since the EGR prevents the NO_x emergence directly in the moment of combustion, it cannot be considered as an exhaust gas aftertreatment technology. Thus EGR will not be included in an exhaust gas aftertreatment configuration selection. However, the following consideration does not dismiss concurrent application of EGR and catalystbased

¹Applies primarily for the SCR catalyst.

CHAPTER 3. CONSIDERATION OF AFTERTREATMENT SYSTEM CONCEPTS 21

aftertreatment technologies. On the contrary, if future emission limits will become prohibitively tight and can not be reached with separate means, the possible solution will likely contain a combination of both EGR and catalytic aftertreatment technologies.

The presence of multiple aftertreatment devices will naturally increase the complexity and subsequently the price of whole aftertreatment system. Therefore all benefits and shortcomings of possible solutions should be considered in a real-world situation. However in this case, adequate simplification will be adopted. Cost and infrastructure-related issues will be disregarded.

The different exhaust gas aftertreatment system concepts are depicted in Figure 3.1.



Figure 3.1: Concepts of combined NO_{x} and DPF exhaust gas after treatment systems [9]

3.2 Comparison of Aftertreatment System Setups

A comparison of aftertreatment system configurations based on the findings presented in [9] is presented below. The aftertreatment systems depicted in Figure 3.1 will be compared regarding important factors such as:

- Low / high temperature activity
- Effort for active DPF regeneration
- Benefit from soot oxidation by NO_2
- Thermal aging
- Risk of sulphur poisoning / effort for desulphurization
- Potential for NO_{x} reduction during DPF regeneration
- Packing demands / system complexity
- Fuel penalty
- Overall NO_x reduction potential

A comparison and assessment of the different concepts of aftertreatment systems, as seen in Table 3.1, shows that there are specific positives and negatives connected with each system configuration. The numbering of aftertreatment system concepts corresponds with the numbering given in Figure 3.1.

The LNT technology is favored when a small aftertreatment system package is required, therefore it is likely to be used in smaller vehicles. Also the LNT is more versatile with regards to a combination with the DPF. The DPF can benefit from heat generated during the LNT NO_x regeneration event [2] in the case of concept No. 3 and partially No. 5. Or if the DPF is placed upstream of the LNT, it can utilize the NO_2 for additional soot oxidation. On the other hand, significant negatives for the LNT exist. The LNT possesses higher susceptibility to thermal aging and sulphur poisoning and it has a lower NO_x reduction potential in comparison with the SCR. Application of the SCR technology results in a more complex aftertreatment system, but it offers more fuel efficient operation unlike the LNT. Unfortunately the SCR has increased demands regarding packing issues, which are mainly related to the additional urea storage tank, and it possesses slightly

Technology	Concept number	High temperature activity	Low temperature activity	Active DPF regeneration	Soot oxidation by NO ₂	Thermal aging	Sulphur poisoning	NO_{x} red. during DPF reg.	Packing/complexity issues	Fuel penalty	NO _x reduction potential
SCD	1	+	—			0	+	++		o/+	+ + +
SUL	2	+		+	+	—	+	—	—	—	+ + +
	3	_	++	0		0			++	0	+
LNT	4	+	_	+	+				+	_	+
	5	+	+	0	0	_		_	+	_	+

Table 3.1: Assessment of concepts for combined DPF and NO_x aftertreatment systems, based mainly on [9]. Legend: '+' positive, 'o' neutral, '-' negative

lower efficiency under a low temperatures compared with the LNT. The major benefit of the SCR technology is its superior overall NO_x reduction potential.

When considering required NO_x conversion rates, specific limitations given by used test cycles as well as the available space on-board the vehicle as determinative factors of the suitable aftertreatment technology and setup selection, the following general trend can be observed [9]: On one side, the SCR technology is a first choice for large vehicles that require high NO_x reduction efficiencies over high kilometrage (such as SUVs for US Tier 2 Bin 5 emission standards or heavy-duty trucks for Euro VI emission standards). On the other side, the LNT technology is considered as an attractive alternative for smaller vehicles with lower demands on NO_x reduction efficiency (e.g. for Euro V emission standards and further). The mentioned trend is depicted in Figure 3.2.

It is obvious that any aftertreatment system configuration has to be addressed with specific decisive factors for individual vehicle application with the emphasis of purpose and vehicle size. The selection of aftertreatment technology has to be supported by thorough simulation of the exhaust aftertreatment system including the temperatures as well as emission concentrations in different driving cycles and for various ambient

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temperature conditions.

NO_x reduction efficiency

Figure 3.2: Common trend for LNT and SCR tech. applications [9]

3.3 Selection of the Aftertreatment System

Since the exhaust gas aftertreatment systems for the heavy-duty automotive applications of diesel engines are the main area of interest of this thesis, the SCR technology will be chosen for further study concerning the modeling and control of an aftertreatment system. When considering SCR technology, there are two SCR aftertreatment system configurations in Table 3.1. Concept No. 2 is less complex and also offers other benefits regarding the DPF regeneration, however it requires substantially more development effort in comparison with SCR concept No. 1 due to interactions between integrated devices. Therefore concept No. 1 is chosen as a reference configuration for aftertreatment model development in the following chapters.

Chapter 4

Complete SCR System Model

In this chapter, a mathematical model of a complete SCR system is described. Firstly, the general problem of the model dimensionality choice and the governing phenomena that take place in a SCR catalyst is discussed. Then follows a description of SCR model structure. Further shown are mass and energy balance equations. The model description is completed by a chemical reaction mechanism, which represents SCR chemistry, and also by reaction rates, which are closely conjoined with presented chemical reactions.

4.1 Model Dimensionality Consideration

Catalytic converters are complex three-dimensional (3D) devices, thus if a rigorous model of such a device is needed, it should be designed as a fully 3D structure. However, running simulations that utilize such a model would be vastly time consuming, not to mention the calibration effort of such a model, which would consume even more time. Hence the 3D model is not suitable for control purposes, where short simulation runs are necessary. Problems with the complexity of modeling a 3D catalyst led to the fact that substantial number of authors, for example [22], [3], [23] and [24], chose a one-dimensional (1D) model, especially for purposes of control research. These 1D models are relatively simple yet still reasonably accurate, fast in terms of computational efficiency and simulation time, and comparatively easy to calibrate. Also, in this case, the 1D model of an aftertreatment system is considered. The thought process of dimension reduction is described further.

The SCR catalytic converter¹ consists of a ceramic monolith with a high amount of

¹Described in detail in 2.1.2

miniature parallel square channels. For simplification, it is assumed that all channels have uniform inlet conditions. Therefore all channels are supposed to be identical. This simplification allows the Cartesian coordinates 3D model to be reduced into a radial coordinates 2D model. Since the longitudinal axes of catalyst channels are parallel to the longitudinal axis of the catalyst, the only relevant difference between 2D and 1D model is a radial heat transfer considered for the 2D model [25]. Thus further reduction of model dimensionality is possible if the radial heat transfer is neglected. Then, consequently, it is possible to shrink the whole 3D system into a single channel model. Obtained is a single channel model consisting of a bulk gas phase and a surface phase, that includes washcoat and underlying ceramic substrate.

4.2 Structure of the Complete SCR Model

The complete SCR model, shown in Figure 4.1, consists of an Oxidation catalyst in close coupled position to the exhaust manifold, intermediate piping with a Urea injection unit and a main SCR catalyst. The lowered subscripts u, m and d represent corresponding locations in relation to the model, namely upstream, middlestream and downstream. Each of the three denoted submodels is modeled in accordance with the important governing phenomena, which are discussed in following section.



Figure 4.1: Complete SCR system model schematic, based on [23]

The SCR submodel presented in the following sections disregards the HC and PM present in exhaust gases, since these species do not affect the main NO and NO_2 reduction pathways [23]. However, the influence of HC and PM has to be taken into account regarding the function of the Oxidation catalyst. This will be done in the simplified way mentioned later.

4.3 Governing Phenomena

The relevant governing phenomena that take place in single channel 1D model are shown in Figure 4.2 and in table 4.1 below.



Figure 4.2: Intra cat. phenomena [26]

No.	Description
1	Bulk flow (gas)
2	Interphase (gas-surface)
3	Chemical reaction (surface)
4	Heat generation (surface)
5	Diffusion through washcoat (s.)
6	Axial heat conduction (surface)

Table 4.1: Intra cat. phenomena [26]

However, the influence of some of the mentioned phenomena may be inferior in comparison with the other. Therefore, not all of the presented phenomena need to be modeled. The effects of pore diffusion through the washcoat are often neglected and lumped into the kinetic rate expressions [27]. Moreover, heat generated through SCR reactions is negligible in comparison with the heat generated through the HC oxidation occurring in the gasoline Three Way Catalyst. Also the effects of axial heat conduction are small when compared with the heat convection through the catalytic converter due to the exhaust gas mass flow.

The reduction efficiency of the catalyst is dependent on three main factors: chemical species, temperature and transit time [25]. Obviously, the catalyst can reduce only specific chemical species. Without proper exhaust gas composition it would not operate as it was intended. Secondly, chemical reactions are temperature dependent in exponential order, thus it is necessary to model the proper temperature behavior of the catalyst. And finally an increased transit time evidently leads to a more complete NO_x reduction, since the chemical processes have more time to run through.

With information provided by the relevant governing phenomena, it is possible to describe an entire catalyst utilizing mass and energy balance equations for both bulk and surface phases present within the single channel 1D model. Mass balance equations are formulated as a set of partial differential equations (PDE). The quantity of PDEs is given by the number of participating chemical species. These equations allow to evaluate relative concentrations of considered chemical species through the device. The energy balance equations are used to model the temperature profile through the model of the catalyst. Both mass and energy balance equations incorporate the residence time within the catalyst through advection terms [25] and are dependent on time and position. Mentioned mass and energy balance equations are widely used in the literature [22], [3], [23], [25] and others.

A summary of governing equations [25] follows:

• Mass balance equations

- Bulk gas species (BGS)
- Surface species (SS)
- Intermediate (adsorbed) species (IS)
- Energy balances
 - Bulk gas temperature (BGT)
 - Surface temperature (ST)
 - Housing temperature (HT)

Interrelations between outlined governing equations are shown in Figure 4.3, where Subfigure 4.3(a) depicts mass balances and Subfigure 4.3(b) depicts energy balances. All stated equations are thoroughly described in the following sections.



(a) Mass balance equations

(b) Energy balance equations

Figure 4.3: Governing equation interrelations for single channel catalyst model

It was mentioned that the both mass and energy balance equations are position dependent. Such equations can be solved using a dedicated solver, e.g. COMSOL multiphysics. Or they can be solved as a set of ODEs while using a finite volume method implemented through spatial discretization. Therefore, in order to solve the PDEs, the OC, intermediate piping and SCR submodels are split into $n_{\rm OC}$, $n_{\rm IP}$ and $n_{\rm SCR}$ identical cells that contain a small fraction of submodels volume². Each control volume is then described by set of ODEs. The PDEs treated this way are comparatively easier to solve. Later, for each written PDE, the corresponding discrete representation is presented.

4.4 Mass Balances

Regarding the mass balance equations, the presented model uses the inference noted in [25]. In this case, the mass balance equations involve a bulk gas species equation, a surface species equation and a surface intermediate species equation. The description of denoted equations is presented below.

It is assumed that a cross-sectional area A_{cs} of the catalyst channel is constant along the entire length of the catalyst. Therefore, the control volume V_c , defined as $V_c = A_{cs}\partial x$, is also constant. Thus it can be replaced by a dimensionless fraction, which is discussed later. This replacement allows each presented mass balance equation to be expressed in units per volume.

4.4.1 Bulk gas species

On the basis of the Euler equation, the following bulk gas species equation for conservation of chemical species on a molar basis is utilized:

$$\varepsilon \frac{\partial C_{\mathrm{g},i}}{\partial t} + u\varepsilon \frac{\partial C_{\mathrm{g},i}}{\partial x} = -k_{\mathrm{m},i}G_{\mathrm{a}}(C_{\mathrm{g},i} - C_{\mathrm{s},i})$$

$$(4.1)$$

The left-hand side of the given equation is according to the common praxis in fluid dynamics denoted as the 1D expression of convective [28] or the Stokes derivative [29]. In our case the first term of the left-hand side stands for the accumulation of species i in gas phase, which is denoted by the lowered subscript g, and the second term on the left-hand

²The so-called control volume

side models a change in concentration of species *i* due to the exhaust gas flow through the catalyst channel in an axial direction. The ε denotes the so-called void fraction, which will be explained further. The exhaust gas flow rate *u* is assumed to be constant³ along the whole catalyst channel and can be computed from the following equation:

$$u = \frac{\dot{m_s}}{\rho_{\rm g} A_{\rm f,s}} \tag{4.2}$$

where $\dot{m_s}$ is an exhaust gas mass flow through corresponding submodel s, ρ_g is an exhaust gas density and $A_{f,s}$ is a frontal flow area of the corresponding submodel. Obviously the u should be indexed by lowered subscript s as should several other variables, however for preservation of clarity, the lowered subscript s is omitted.

Finally, the first term on the right-hand side of equation 4.1 stands for mass transfer through diffusion from/to the surface of the catalyst, where $k_{m,i}$ is the mass transfer coefficient of species *i*. The G_a denotes a geometric surface area-to-volume ratio for a square/circular catalyst channel. The G_a can be defined by the following expression:

$$G_{\rm a} = \frac{4\varepsilon}{d_{\rm m}} \tag{4.3}$$

where the $d_{\rm m}$ stands for the hydraulic diameter of the catalyst channel and ε represents the previously mentioned void fraction, which can be written as follows:

$$\varepsilon = \frac{V_{\rm g}}{V_{\rm cat}} \tag{4.4}$$

The void fraction denotes the fraction of catalyst volume⁴, which is accessible for bulk gas. Thus expression $1 - \varepsilon$ essentially means the fraction of the catalyst volume that is occupied by the monolith.

When a spatial discretization through backward differences is applied, the Equation 4.1 can be rewritten as follows:

$$\varepsilon \frac{\mathrm{d}C_{\mathrm{g},i,j}}{\mathrm{d}t} + u\varepsilon \frac{(C_{\mathrm{g},i,j} - C_{\mathrm{g},i,j-1})}{\Delta x} = -k_{\mathrm{m},i}G_{\mathrm{a}}(C_{\mathrm{g},i,j} - C_{\mathrm{s},i,j}) \tag{4.5}$$

³Actually it is an approximation. Change of gas moles on product side, as seen in chemical reactions in subsection 4.6.1, is neglected. Its influence on u is minimal due to the relatively small amount of reaction products in exhaust gas.

⁴There are certain differences in the void fraction value for OC and SCR catalytic converters

where Δx represents a length of segment j of the corresponding submodel. The index j has values $0, ..., n_k$ where $n_k \in \{n_{\text{OC}}, n_p, n_{\text{SCR}}\}$ depending on the current submodel. The concentration with index i = 0 denotes the catalyst inlet boundary conditions in the first submodel cell.

4.4.2 Surface Species

The chemical species transferred from bulk gas to porous monolith washcoat, where the catalytically active metal is present, are subject to the mass conservation equation:

$$(1-\varepsilon)\frac{\mathrm{d}C_{\mathrm{s},i}}{\mathrm{d}t} = k_{\mathrm{m},i}G_{\mathrm{a}}(C_{\mathrm{g},i} - C_{\mathrm{s},i}) \pm G_{\mathrm{cat}}\sum_{k}\sigma_{k}r_{k}$$
(4.6)

The left-hand side term represents the accumulation of species i in the porous washcoat at the catalyst surface, which is denoted by the lowered subscript s. Note that accumulation takes place only in the fraction of the catalyst volume defined by the term $1 - \varepsilon$. Further, the first term on the right-hand side stands for mass transfered through diffusion from bulk gas phase to washcoat. It is the same term presented in equation 4.1. The second term incorporated on the right-hand side accounts for the occurrence of chemical reactions at the surface with the adequate active catalytic surface area G_{cat} and the stoichiometric coefficient $\sigma_{i,k}$. The sign of the reaction term depends on whether the reaction consumes or produces the corresponding chemical species. Complete definition of reaction rate r_k will be presented later in 4.6.2.

It should be mentioned, that equation 4.6 disregards the effect of the slip boundary condition on the surface of the catalyst [25], therefore axial velocity of the surface species is neglected. Another major simplification is possible owning to the fact that the accumulation of species in the surface is significantly smaller in comparison to the other phenomena; typically reaction rates are much larger in magnitude. Therefore the corresponding term can be omitted. Then the surface species equation can be rewritten in form of an algebraic equation:

$$k_{\mathrm{m},i}G_{\mathrm{a}}(C_{\mathrm{g},i} - C_{\mathrm{s},i}) = \pm G_{\mathrm{cat}}\sum_{k}\sigma_{k}r_{k}$$

$$(4.7)$$

An observant reader should notice that the surface mass transfer term present in equation 4.1 can be substituted by the right-hand side term of the above mentioned equation. Therefore both the bulk gas species and the surface species equations can be joined together resulting in:

$$\varepsilon \frac{\partial C_{\mathrm{g},i}}{\partial t} + u\varepsilon \frac{\partial C_{\mathrm{g},i}}{\partial x} = \pm G_{\mathrm{cat}} \sum_{k} \sigma_{k} r_{k}$$
(4.8)

When applying the spatial discretization to equation 4.8, the resulting equation for both gas and surface mass balances can be written as follows:

$$\varepsilon \frac{\mathrm{d}C_{\mathrm{g},i,j}}{\mathrm{d}t} + u\varepsilon \frac{(C_{\mathrm{g},i,j} - C_{\mathrm{g},i,j-1})}{\Delta x} = \pm G_{\mathrm{cat}} \sum_{k} \sigma_k r_k \tag{4.9}$$

4.4.3 Intermediate Species

Generally, the surface reaction mechanisms are very complex and therefore are not fully understood yet. In order to simplify modeling effort researchers have begun to use 'quasielementary' steps to describe actual reactions occurring on the molecular level [25]. These reactions involve gaseous species and precious metal species present on the catalyst surface. Intermediate species are widely used in the literature for modeling primarily the adsorption/desorption of gases onto the reaction sites on the surface. Various reactions occur at the surface involving numerous combinations of gas and intermediate species. Moreover, there could be more than one type of adsorption site on the surface. Various gas species could compete for available adsorption sites. Also, the catalyst is susceptible to deactivation and aging, which leads to the loss of adsorption sites. All mentioned above is is described by the general surface intermediate coverage equation [30].

For the purpose of developing a simple aftertreatment system model, several assumptions have to be adopted in accordance with current literature. The SCR catalytic converter can be modeled accurately while considering only gaseous ammonia as capable of forming surface intermediate species. Further all adsorption sites are assumed to be equal and no potential loss or gain of adsorption sites takes place through catalyst aging and deactivation. Moreover one gas molecule can occupy exactly one adsorption site. Thus the ammonia intermediate species surface coverage equation can be written as follows:

$$\frac{\mathrm{d}\theta_{\mathrm{NH}_3}}{\mathrm{d}t} = \frac{1}{L_{\mathrm{Pt}}} \sum_k \sigma_k r_k \tag{4.10}$$

The given equation represents production/consumption of ammonia surface intermediates through ammonia surface coverage $\theta_{\rm NH_3}$, which is dependent on the sum of the products of stoichiometric coefficients σ_k and reaction rates r_k and therefore on corresponding reactions, where the NH₃ intermediate is consumed or produced. The denominator $L_{\rm Pt}$ stands for the density of platinum adsorption sites on the catalyst surface.

The equation 4.10 is ODE and it should be solved implicitly due to stiffness issues [25]. The spatial discretization of equation 4.10 is not necessary, since it can be quantified for every catalyst segment j separately.

Adsorption and desorption occur also in the Oxidation catalyst, where one of the involved chemical species is oxygen. Moreover, the adsorption sites of the Oxidation catalyst surface can be occupied by numerous chemical compounds, especially HC and soot. Thus the oxygen has to compete for available free sites. However, the corresponding reaction could be modeled accurately without implementing intermediate species [31] by a properly written reaction rate, which is mentioned further in 4.6.2. The presented surface intermediate reaction mechanism enables usage of relatively detailed chemical reactions in the catalyst model.

4.5 Energy Balances

The chemical reactions occurring in the catalytic converter are naturally highly dependent on the exhaust gas temperature. Therefore the subject of study in this section is energy balances in the catalyst. The energy balance equations describe heat transfer processes in each of submodels. The energy balances are defined for both catalytic converters and for intermediate piping. Corresponding equations, namely bulk gas temperature, surface temperature and housing temperature, are presented in this section.

4.5.1 Bulk Gas Temperature

The temperature of bulk gas can be expressed as the following equation:

$$\varepsilon \rho_{\rm g} c_{\rm p,g} \frac{\partial T_{\rm g}}{\partial t} + \varepsilon \rho_{\rm g} c_{\rm p,g} u \frac{\partial T_{\rm g}}{\partial x} = -h_{g \to m} G_{\rm a} (T_{\rm g} - T_{\rm m})$$
(4.11)

The first left-hand side term stands for the accumulation of heat in control volume. This is defined as a product of the void fraction ε , the exhaust gas density $\rho_{\rm g}$, an exhaust gas specific heat capacity $c_{\rm p,g}$, and a temperature of exhaust gas $T_{\rm g}$. The second term on the left-hand side denotes the main heat source of the catalytic converter; the heat convection by the exhaust gas mass flow through the device. The first term on the right-hand side denotes the inter-phase heat transfer from gas to monolith, where the $h_{\rm g\to m}$ stands for the conductive heat transfer coefficient between bulk gas and monolith according to Newton's law of cooling.

The corresponding spatial discretization of equation 4.11 follows:

$$\varepsilon \rho_{\rm g} c_{\rm p,g} \frac{\mathrm{d}T_{\mathrm{g},j}}{\mathrm{d}t} + \varepsilon \rho_{\rm g} c_{\rm p,g} u \frac{(T_{\mathrm{g},j} - T_{\mathrm{g},j-1})}{\Delta x} = -h_{g \to m} G_{\rm a} (T_{\mathrm{g},j} - T_{\mathrm{m},j}) \tag{4.12}$$

4.5.2 Surface Temperature

Since the monolith represents the solid-phase in the catalytic converter, its temperature determines how fast or slow the surface reactions will take place. The monolith temperature can be described by the following equation:

$$(1-\varepsilon)\rho_{\rm m}c_{\rm p,m}\frac{\partial T_{\rm m}}{\partial t} = h_{g\to m}G_{\rm a}(T_{\rm g} - T_{\rm m}) - Q_{\rm m\to h}$$

$$(4.13)$$

This equation presents the dependency of monolith temperature on heat transferred from gas phase and on heat transferred to the catalyst housing. The first term on the lefthand side stands for heat accumulation in the monolith, where $\rho_{\rm m}$ denotes a density of monolith material and $c_{\rm p,m}$ is a specific heat capacity of monolith material. Note that the first term on the right-hand side is the same as in equation 4.11. The remaining term on the right-hand side of equation 4.13 is the conductive heat transferred from monolith to housing, $Q_{\rm m \rightarrow h}$ and can be expressed by the following equation:

$$Q_{\mathrm{m}\to\mathrm{h}} = k_{\mathrm{m}\to\mathrm{h}} A_{\mathrm{h,in}} (T_{\mathrm{m}} - T_{\mathrm{h}})$$

$$(4.14)$$

where $k_{m \to h}$ represents the heat conduction transfer coefficient between monolith and housing and $A_{h,in}$ stands for the surface of inner catalyst housing wall, which is in contact with the monolith.

The spatial discretization of equations 4.13 and 4.14 is not necessary, hence these

equations can be easily quantified for each of the spatial catalyst segments by substituting corresponding temperatures.

4.5.3 Housing Temperature

In addition to the energy balance governing equations, which includes the bulk gas temperature and the surface temperature, another equation is introduced to the model. It represents the heat transfer from monolith to the catalyst housing and subsequently to the ambient environment. This equation should be seen as a supplementary extension of the surface temperature balance equation, since it is assumed for simplification that the monolith is housed directly in a metal can. The influence of the intumescent mat, mentioned in 2.1.2, is disregarded. The housing temperature equation can be written as:

$$m_{\rm h}c_{\rm p,h}\frac{\partial T_{\rm h}}{\partial t} = Q_{\rm m \to h} - Q_{\rm h \to a} \tag{4.15}$$

where $m_{\rm h}$ is a mass of a catalyst housing and $c_{\rm p,h}$ is a specific heat capacity of a catalyst housing material. The term $Q_{\rm h\to a}$ stands for a heat transferred from the catalyst housing to outer ambient environment and it is defined by the following equation:

$$Q_{\rm h\to a} = \varepsilon_{\rm h} \sigma A_{\rm h,out} (T_{\rm h}^4 - T_{\rm a}^4) + k_{\rm h\to a} A_{\rm h,out} (T_{\rm m} - T_{\rm h})$$

$$\tag{4.16}$$

The first term on the right-hand side stands for radiation, where $\varepsilon_{\rm h}$ is an emissivity of a catalyst housing outer wall, σ is the Stephan-Boltzman radiation constant and $A_{\rm h,out}$ is a surface of outer catalyst housing wall. The remaining term on the right-hand side represents a conductive heat transfer, where $k_{\rm h\to a}$ is a heat conduction transfer coefficient between the housing and the ambient environment. Note that the heat radiation is comparatively inferior, especially under lower temperature conditions, when compared to the heat conduction. However, amount of the heat transfered through the heat radiation increases with the fourth power of the temperature, thus for temperatures exceeding 450 °C, it cannot be neglected. Also in a case of equation 4.15 the spatial discretization is not necessary.

If greater fidelity of exhaust gas aftertreatment model behavior is needed, the exhaust gas aftertreatment model can be extended by the currently disregarded intumescent mat or even by an insulation layer to obtain more accurate results.

4.6 Reaction Mechanism

Generally, a reaction mechanism describes how the chemical reactions occur. All considered chemical reactions take place on the washcoat surface of the catalyst in presence of active catalytic species. Thus they don't take place directly in the bulk gas volume. There are two different reaction mechanisms for the surface reactions in the literature, typically Langmuir-Hinshelwood (LH) or Eley-Rideal (ER). The LH reaction mechanism assumes parallel adsorption of two different chemical species on the surface. The chemical reaction occurs on the surface under the condition that both species have diffused sufficiently close to one another. Unlike the LH reaction mechanism, the ER reaction mechanism supposes adsorption of only one chemical species on the surface. Thus the chemical reaction is taking place by access of reactants directly from gas to adsorbed species on the surface. In case of the SCR catalyst, many authors [23], [3], [22] prefer the ER reaction mechanism, since the only species adsorbed on surface is the NH₃.

Chemical reactions and corresponding reaction rates associated with reduction processes taking place in a catalytic converter are discussed in this section. Chemical reactions presented in the following subsection are implemented in the aftertreatment system model.

4.6.1 Chemical Reactions

The most significant chemical reactions that are taking place in the SCR aftertreatment system are presented below.

Urea decomposition is modeled by following equation:

$$(\mathrm{NH}_2)_2\mathrm{CO} + \mathrm{H}_2\mathrm{O} \longrightarrow 2\,\mathrm{NH}_3 + \mathrm{CO}_2$$
 (4.17)

Gaseous ammonia, which is formed from urea decomposition is further adsorbed on the surface⁵ of the SRC catalyst. However, the desorption also takes place in the catalyst, particularly under higher temperature conditions, and has to be taken into account.

$$\mathrm{NH}_3 + ^* \rightleftharpoons \mathrm{NH}_3^*$$
 (4.18)

 $^{^5 \}mathrm{The}$ * stands for an adsorption site.

Oxidation of ammonia is determined by:

$$4 \operatorname{NH}_{3}^{*} + 3 \operatorname{O}_{2} \longrightarrow 2 \operatorname{N}_{2} + 6 \operatorname{H}_{2} \operatorname{O}$$

$$(4.19)$$

This reaction takes place at temperatures exceeding 450 °C, which is outside of the optimal operating temperature window of the SCR catalyst. Under that condition ammonia is desorbed and oxidized directly into nitrogen.

The selective catalytic reduction is modeled by the following three equations. The consumption of adsorbed ammonia, gaseous NO and NO_2 is considered while employing the Eley-Rideal reaction mechanism:

$$2 \operatorname{NH}_{3}^{*} + \operatorname{NO} + \operatorname{NO}_{2} \longrightarrow 2 \operatorname{N}_{2} + 3 \operatorname{H}_{2} \operatorname{O}$$

$$(4.20)$$

$$4 \operatorname{NH}_{3}^{*} + 4 \operatorname{NO} + \operatorname{O}_{2} \longrightarrow 4 \operatorname{N}_{2} + 6 \operatorname{H}_{2} \operatorname{O}$$

$$(4.21)$$

$$8 \operatorname{NH}_{3}^{*} + 6 \operatorname{NO}_{2} \longrightarrow 7 \operatorname{N}_{2} + 12 \operatorname{H}_{2} \operatorname{O}$$

$$(4.22)$$

The first equation, often denoted as a fast SCR reaction, is the most desirable, since it reduces both NO and NO₂ more rapidly than other two reactions. Regarding this chemical reaction, the NO to NO₂ ratio should not be less than one in order to minimize effects of comparatively slower reactions [23]. The second equation is called a standard SCR reaction. Besides NO and NH₃, it is also dependent on the presence of O₂. However, this dependence is often neglected in the literature [23], since the O₂ is far more abundant in exhaust gas unlike NO. The last equation, denoted as a SCR NO₂ reaction, is the slowest among all three SCR reactions considered. Therefore, its influence on total NO_x reduction efficiency is minor.

It has been noted in 2.1.3, that 90% of the deisel engine NO_x output is the NO. Since the reaction 4.20 is the most desirable, it is necessarry to reduce part of the NO exhaust gas content to obtain 50/50 mixture of NO and NO_2 . This is done by utilizing the Oxidation catalyst, where the following chemical reaction occurs:

$$2 \operatorname{NO} + \operatorname{O}_2 \longrightarrow 2 \operatorname{NO}_2$$

$$(4.23)$$

This reaction takes place in both directions, however the dynamic equilibrium is rather on the product side under conditions that occur in the Oxidation catalyst. Therefore the reversibility of this reaction is neglected. For interested readers, cutting edge research of NO oxidation is available in [31]. Additionally, all remaining given chemical equations are considered to have a dynamic equilibrium far on the product side, therefore only forward reactions are taken into account. The only exception is the ammonia adsorbtion/desorbtion reaction, for which a proper dynamical equilibrium has to computed for given temperature conditions, since ammonia presence on the catalyst surface has a major impact on the SCR reduction processes.

4.6.2 Reaction Rates

The reaction rate defines how fast the chemical reaction consumes reactants and produces products. Generally, reaction rate can be expressed as the following equation:

$$r_k = \frac{\mathrm{d}C_k}{\mathrm{d}t} = k_k \prod_i C_i^{\sigma_i} \tag{4.24}$$

The reaction rate r_k of reaction k is, in fact, a rate of a concentration change in time. It depends on a rate constant k_k and on the product of concentrations C_i of all involved chemical species *i*, where σ_i is the stoichiometric coefficient of the corresponding species.

However the rate constant is not actually constant, but it is temperature dependent. There are two distinct derivations of the rate constant used in the literature. The first widely used derivation of rate constant is the Arrhenius law, that can be written as:

$$k_k = A_k \exp\left[\frac{-E_{\mathrm{a},k}}{RT_{\mathrm{m}}}\right] \tag{4.25}$$

where A_k is a pre-exponential factor of reaction k, $E_{a,k}$ stands for an activation energy, R is a gas constant and finally T_m is the temperature of a catalyst monolith. The Arrhenius type reaction rate assumes an ideally stirred reaction environment.

The rate constant, especially for an adsorption (bimolecular) reaction, can be derived differently using ideas of statistical thermodynamics [32] by computing the number of collisions of gas particles on the catalyst surface per time and catalyst area [23]. The corresponding formula can be written as:

$$k_k = \frac{1}{L_{\rm Pt}} \frac{s}{\sqrt{2\pi M_i R T_{\rm g}}} \tag{4.26}$$

where s is a sticking probability, which expresses the number of collisions that actually lead to a reaction, M_i is a molar mass of species i and T_g is a gas temperature. This type of reaction rate is assumed to be diffusion driven.

When comparing both manners of the rate constant derivation, the second one describes catalytic reactions more accurately but can be reasonably used only for bimolecular reactions since it has serious difficulties when describing multi-molecular reactions. The first mentioned derivation manner does not suffer from the mentioned disadvantage, therefore its utilization is preferred for the SCR model implemented in this thesis.

Chapter 5

Validation of the Aftertreatment System Model

A validation of the aftertreatment system model is presented in this chapter. First of all each of three submodels is independently put through a series of simulations whose results are evaluated against anticipated outcomes. Additionally, the influence catalyst parameter values on catalyst function are studied in order to obtain basic knowledge of possible submodel performance improvements by altering proper catalyst parameter values.

Since any major simplifications have not taken place yet, the submodels contain very fast and slow dynamics. Especially the fast dynamics cause severe problems due to dynamic stiffness issues when using direct numerical simulation solvers such as ode45 or ode23 in MATLAB. Thus different solver has to be used to improve numerical stability of the simulation. The ode15s proved itself to be a suitable solution.

5.1 Oxidation Catalyst

The Oxidation catalyst submodel is evaluated first. This submodel is based on equations introduced in chapter 4 and is implemented by using the Level-2 M-File S-Function in MATLAB. The function of the Oxidation catalyst has been presented in subsection 2.2.2, however it may be appropriate to recall the purpose of OC. Essentially, the OC changes the NO/NO₂ ratio to approximately 50/50 since the NO represents almost 90% of total engine NO_x output. The proper mixture of individual NO_x in the exhaust gas is fun-

damental to achieving maximal NO_x reduction efficiency of the downstream-placed SCR catalyst. Therefore, instead of absolute NO_x concentrations, the most important characteristics of OC, in view of SCR function support, are the NO_x ratios. Values of NO_x ratios are mostly dependent on inlet gas temperature. The temperature dependency can be clearly seen through the NO_x chemical reaction. It is obvious that influence of different catalyst parametres on the catalyst temperature behavior and on the temperature dependency of NO_x ratios has to be studied and understood.

A set of constant input parameters, given in Table 5.1, is used for all static characteristic simulations in 5.1.1 and in 5.1.2. However, the input parameters are subject to change, since they depend on current operating conditions of vehicle. The impact of their change on catalyst behavior is studied in transient response simulations in 5.1.3.

Input parameter	Value	Input parameter	Value
Concentration of O_2	8000 ppm	Exhaust gas mass flow	0.04 kg/s
Concentration of NO	600 ppm	Ambient temperature	$26.85~^\circ\mathrm{C}$
Concentration of NO_2	60 ppm	Exhaust gas pressure	101 kPa

Table 5.1: Oxidation catalyst input parameters

5.1.1 Basic Static Characteristics

Basic simulations include temperature static characteristics and NO_x ratios static characteristics. The simulations were carried out for catalyst cell length 1 cm. The results of these simulations are presented in the below given figures.



Figure 5.1: Dependence of static char. of $T_{\rm g,out}$, $T_{\rm m,out}$ and $T_{\rm h,out}$ on $T_{\rm g,in}$

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Figure 5.1 depicts a static characteristic of outlet temperatures $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ dependence on inlet exhaust gas temperature $T_{g,in}$. The steady state outlet exhaust gas, monolith and housing temperatures increase linearly for increasing inlet exhaust gas temperature. Note that the monolith has almost the same temperature as the exhaust gas outgoing from an individual submodel segment. The gap between temperatures $T_{g,out}$ and $T_{h,out}$ is naturally widening for rising inlet gas temperature $T_{g,in}$, since the heat losses to the ambient environment depend on he difference of ambient and inner gas temperatures. The contribution of radiative heat losses is negligible, particularly under low temperature conditions, because of any significant slope change visible in $T_{h,out}$.



Figure 5.2: Dependence of static char. of NO_x ratios on $T_{g,in}$

The static characteristic of NO_x ratios' dependence on inlet exhaust gas temperature $T_{g,in}$ is shown in Figure 5.2. The initial state correspond with 10% of NO₂ and 90% of NO₂ content in exhaust gas. The steady state NO ratio drops as the NO conversion increases because of a rise in catalyst temperature. The optimal SCR NO_x reduction point is reachable, while the OC is working in/or near the optimal NO conversion point, because the maximum of the NO_x can be consumed by the fast SCR reaction 4.20. The optimal NO conversion point is defined for a 1:1 mixture of NO and NO₂. However, the optimal SCR NO_x reduction point is not always reachable due to variable temperature conditions. In that case, it is desirable to maintain NO conversion in the zone of higher NO content as seen in Figure 5.2, since the standard SCR reaction 4.21 is faster than the NO₂ SCR reaction 4.22.

The possibilities for the shifting of the optimal NO conversion point for the Oxidation catalyst are analyzed in the second part of following subsection.

5.1.2 Effect of Catalyst Parameters on Static Characteristics

Examples of several physical parameters that are used in the Oxidation catalyst submodel are given in Table 5.2.

Parameter	Value	Parameter	Value
Monolith density	$2~650~\mathrm{kg/m^3}$	Housing density	$8\ 000\ \mathrm{kg/m^3}$
Monolith thermal cond.	$1.7 \mathrm{W/(m K)}$	Housing thermal cond.	$16 \mathrm{W/(m K)}$
Monolith heat capacity	see footnote ¹	Housing heat capacity	510 J/(kg K)
Heat convection to amb.	$50 \mathrm{W/(m K)}$		
# of OC cells	10	Cell length	0.01 m
OC housing outer diam.	0.2 m	Catalyst length	0.1 m
Active cat. surf. area	$5 \ 670 \ m^2/m^3$	Void fraction	0.6836
Channel hydraulic diam.	$0.0016 {\rm m}$	Reaction site density	0.045 mol/m^2

Table 5.2: Oxidation catalyst physical parameters

The first four rows of Table 5.2 contain the first set of parameters that occur in energy balance equations, they affect the temperature behavior of the catalyst. The second set of parameters given in the last four rows of Table 5.2 occur in equations relating to catalyst chemistry, thus they affect NO_x ratios. Note that the monolith material heat capacity is temperature dependent¹, thus it can't be treated as a single parameter.

The experiments are carried out in following manner: singe simulation uses constant inlet exhaust gas temperature of values from 100 °C to 460 °C with step of 20 °C. Every following simulation run uses a higher inlet gas temperature than the previous one. The chosen temperature range covers a substantial part of real-world exhaust gas temperatures. For every simulation run, the studied parameter is set from 70% to 130% of its default value given in Table 5.2 with a step of 15%; remaining parameter values are kept intact. The reason for such step selection is that the parameter influence can be compared easily without need of any additional normalization. Moreover $\pm 30\%$ parameter value fluctuation is reasonably high to cover various Oxidation catalyst configurations. Exception from the $\pm 30\%$ value change rule is the number of OC cells, which has a particular set of values². Any possible cross-sensitivities of change between different parameters is neglected. Finally, the simulation results are collected and steady state values are

¹The monolith heat capacity is defined as $1071 + 0.156 \times T_{\rm m} - 3435 \times 10^4 / T_{\rm m}^2 \text{ J/(kg K)}$

 $^{{}^{2}}n_{\rm OC} \in \{1, 2, 3, 4, 6, 10\}$ with default value $n_{\rm OC, def} = 10$

diplayed in static characteristic figures.

The static characteristics for particular parameter values are distinguished by different line widths in corresponding figures. The wider the chart line, the higher the studied parameter value. This approach ensures better visual readability of presented data.

5.1.2.1 Thermal Static Characteristics

As it is shown in Figure 5.3, the higher the value of the heat conduction transfer coefficient between housing and ambient $k_{h\to a}$, the more heat escapes to ambient environment and the lower is the steady state temperature of the catalyst housing. The steady state temperatures $T_{g,out}$ and $T_{m,out}$ are minimally affected.



Figure 5.3: Dependence of static characteristic of $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ on $T_{g,in}$ and $k_{h\to a}$

Any other significant change in steady state output temperatures is observable for the remaining experiments. Corresponding thermal static characteristics are not presented, since the are available on the attached CD. The effect of change of Oxidation catalyst parameters on thermal static characteristics is rather small, since the convective heat losses to ambient environment are the only modeled heat sink.

5.1.2.2 Static Characteristics of NO_x Ratios

Simulation has revealed some particular NO_x ratios dependencies on Oxidation catalyst parameters. The most important information, from the point of view of aftertreatment control, can be obtained from Figure 5.4, which depicts the dependency of NO_x ratios on a varying number of Oxidation catalyst cells n_{OC} . As expected, the higher number of cells used in a model, the more NO is reduced under low temperature conditions. Thus the optimal NO reduction point moves to the left. However, the length of the whole catalyst is constant, thus the individual cell length decreases for increasing $n_{\rm OC}$. In fact, the $n_{\rm OC}$ determines the actual order of the submodel. Although the NO_x ratios do not change significantly for $n_{\rm OC} = 4$ and higher, the default $n_{\rm OC}$ is left intact for the rest of the simulations. Obviously, more simulation effort and comparison with real data is necessary to obtain more precise information about sufficiently high n_{OC} for practical use in control.



Figure 5.4: Dependence of static characteristic of NO_x ratios on $T_{g,in}$ and n_{OC} , $(n_{OC} \in \{1, 2, 3, 4, 6, 10\}, n_{OC,def} = 10)$

The optimal NO conversion point position is mostly dependent on Oxidation catalyst dimensions, i.e. housing diameter $d_{h,OC}$ and Oxidation catalyst length x_{OC} as it is shown in Figures 5.5 and 5.6.



Figure 5.5: Dependence of static char. of NO_x ratios on $T_{g,in}$ and $d_{h,OC}$

Figure 5.5 depicts the dependency of NO_x ratios static characteristic on inlet gas

temperature $T_{g,in}$ and catalyst housing diameter $d_{h,OC}$. With increasing diameter and thus with increasing catalyst volume more NO present in exhaust gas is reduced under lower temperature conditions.



Figure 5.6: Dependence of static char. of NO_x ratios on $T_{g,in}$ and x_{OC}

A similar situation takes place when considering Figure 5.6, where the dependence of NO_x ratios static characteristic on inlet gas temperature $T_{g,in}$ and length of catalyst segment x_{OC} is shown. However, the effect of increasing catalyst length is lower because of smaller volume gain. Naturally, the Oxidation catalyst size plays a significant role in catalyst function. This is in accordance with real-world observations, where bigger a catalyst can usually convert more pollutants than a smaller one.

The following figures depict the influence of monolith and washcoat parameters on steady state NO_{x} ratios.



Figure 5.7: Dependence of static char. of NO_{x} ratios on $T_{\mathrm{g,in}}$ and ε

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The dependency of the static characteristic of NO_x ratios on inlet gas temperature and void fraction ε is shown in Figure 5.7. Interesting is the fact that the increasing void fraction actually lowers NO conversion at a given temperature. This can be explained that if more space is available for exhaust gas in the monolith at constant $L_{Pt,OC}$, the more the reaction sites are diluted across the catalyst and the less NO is converted, because of a comparatively low concentration of NO_x in exhaust gas.

Figures 5.8 and 5.9 depict NO_x ratios dependency on temperature as well as on important washcoat parameters such as surface-to-volume area G_{cat} , platinum metal loading and the reaction site density $L_{Pt,OC}$. Clearly, the usage of monolith washcoat with properly engineered parameters allows the catalyst manufacturer to fine-tune the desired location of the optimal NO conversion point. Note that the mentioned parameters have almost equal impact on OC function according to the pictures.



Figure 5.8: Dependence of static char. of NO_x ratios on $T_{g,in}$ and G_{cat}



Figure 5.9: Dependence of static char. NO_x ratios on $T_{g,in}$ and $L_{Pt,OC}$

5.1.3 Transient Response Dynamic Characteristics

The step of $T_{g,in}$ from 30 °C to 300 °C at time 0 s has been used for the transient response characteristics simulation. Influence of parameter changes on thermal, NO_x ratios and input variables transient response characteristics are presented in this subsection. The studied parameters are changed in a range of ±30%, the same as in subsection 5.1.2.

5.1.3.1 Thermal Transient Responses

First of all, several of the most significant temperature transient response characteristics are presented in the following figures. The remaining figures of temperature transient characteristics can be found on the attached CD.

Figure 5.10 depicts the influence of varying n_{OC} on the temperature dynamics of the catalyst. A slowdown in temperature dynamics is observable particularly for lower n_{OC} values. For n_{OC} higher than 4 is the change negligible. Another fact can be seen from this figure. The n_{OC} does not significantly affect the steady state outlet temperatures, which goes along with the findings from static characteristic presented in subsection 5.1.2.1.



Figure 5.10: Transient response of $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ for various n_{OC} , $(n_{OC} \in \{1, 2, 3, 4, 6, 10\}, n_{OC,def} = 10)$

The outlet temperature transient response for various $d_{h,OC}$, and thus for various catalyst sizes, is depicted in Figure 5.11. The results show, that for the larger catalyst it takes more time to warm up. This corresponds to real catalyst behavior. Also the difference of outlet gas and monolith temperature decreases, due to greater heat transfer from gas to monolith, relating to the size of the catalyst.



Figure 5.11: Transient resp. of $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ for various $d_{h,OC}$

The outlet temperature transient response for various ε is shown in Figure 5.12. Here the higher void fraction ε significantly decreases the warm up time. More monolith volume becomes accessible for exhaust gas as the ε increases, thus the heat exchange takes place faster than under low ε conditions. This finding can be used by catalyst manufacturers for an adjustment of warm-up time, when faster warm-up is needed. As is previous cases, the ε don't affect the steady state outlet temperatures of the catalyst.



Figure 5.12: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$ and $T_{\rm h,out}$ for various ε

The washcoat parameters, G_{cat} and $L_{\text{Pt,OC}}$, do not affect the temperature dynamics of the catalyst at all, since they are not present in energy balance equations. The monolith and housing thermal conductivities, k_{m} and k_{h} , doe not affect the temperature dynamics of the catalyst either. It may be caused by relatively low values of those parameters.



Figure 5.13: Transient response of $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ for various $c_{p,m}$

The monolith heat capacity $c_{p,m}$ and monolith density ρ_m affect the temperature dynamics significantly as it is shown in figures 5.13 and 5.14. The higher $c_{p,m}$ and ρ_m are, the more heat is required from exhaust gas to warm up the catalyst to a certain temperature - this takes more time. The housing heat capacity $c_{p,h}$ and density ρ_h have similar but smaller scale influence on temperature dynamics. None of mentioned parameters have influence on steady state temperatures.



Figure 5.14: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$ and $T_{\rm h,out}$ for various $\rho_{\rm m}$

The only parameter able to change the steady state temperatures is the heat convection from housing to ambient environment coefficient $k_{h\to a}$. The corresponding transient response is shown in Figure 5.15. The higher the $k_{h\to a}$ is, the more that heat is dissipated to ambient, thus the steady state housing temperature falls. The finding corresponds with the observation presented in subsection 5.1.2.1.



Figure 5.15: Transient response of $T_{g,out}$, $T_{m,out}$ and $T_{h,out}$ for various $k_{h\to a}$

5.1.3.2 Transient Responses of NO_x Ratios

The influence of selected parameters on transient response characteristics of NO ratios is studied in this subsection. Interested readers will find the rest of the transient response characteristics on the attached CD.

There are NO_x ratios transient responses for varying number of OC cells n_{OC} depicted in Figure 5.16. The value of n_{OC} substantially affects the dynamic of NO_x ratios. The more OC cells are present, the less time is needed for reaching particular NO conversion. This is connected to a more complete conversion process through usage of more catalyst cells, which describe the real device more precisely.



Figure 5.16: Transient response of NO_x ratios for various n_{OC}

Note that the values of NO_x ratios steady states are affected as well. The more cells used, the more precise the steady state NO_x ratios that are obtained. The differences

between steady state values of NO_x ratios are 18.7%, 9.2%, 5.6%, 3.6% and 1.7% for $n_{\rm OC} = 1, 2, 3, 4$ and 6 respectively, in comparison with NO_x ratios steady state value for $n_{\rm OC} = 10$ and for an inlet gas temperature step of 300 °C.



Figure 5.17: Transient response of NO_x ratios for various $d_{h,OC}$

The effects of varying catalyst housing diameter $d_{h,OC}$ on the NO_x ratios dynamics are possible to observe in Figure 5.17. The higher the $d_{h,OC}$ value is, the more NO is converted in steady state and the slower the conversion takes place. An analogous situation exists for x_{OC} , although its effects are comparatively lower than the effects of the $d_{h,OC}$.



Figure 5.18: Transient response of NO_x ratios for various ε

Also the monolith parameters contribute to the shape of NO_x ratios dynamics. The most significant influence is observable in case of the void fraction. The corresponding transient responses of NO_x ratios are shown in Figure 5.18. The higher the ε is, the faster the conversion process takes place. However, a decrease in steady state values of NO_x ratios is visible due to more volume accessible to exhaust gas and lower resident time.

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Finally, the NO_x ratios dynamics can be influenced by altering the monolith parameter values. This is shown in Figure 5.19, where the studied parameter is the monolith heat capacity $c_{p,m}$. This parameter substantially affects the rise time of the NO_x ratios. The higher the monolith heat capacity is, the slower the transient response takes place. This is caused by slow temperature dynamics due to a bigger heat reservoir being filled.



Figure 5.19: Transient response of NO_x ratios for various $c_{p,m}$

Unlike the monolith parameters, the housing parameters, such as $c_{p,h}$, ρ_h and $k_{h\to a}$, do not affect the NO_x ratios transient response, since the housing is not directly connected with reaction surface (monolith) temperature.

5.1.3.3 Input Variable Transient Responses

Transient responses of temperature and NO_x ratios of Oxidation catalyst to step change of input variables as seen in Table 5.1 for selected operating points are studied in this subsection.

A step change is introduced via a single input variable per one simulation, with the remaining input variables are left unchanged. In this manner, it is possible to observe the influence of individual input variables on catalyst transient behavior. Also the Oxidation catalyst parameters from Table 5.2 are set on their default values.

The selected operating points OPs, given in Table 5.3, are defined by particular values of $T_{g,in}$ and m_f . Actually, this definition of operating points is simplified, since a complete state of OC is defined by a full set of input variables and operating conditions. However, some operating conditions can be difficultly affected from control point of view, e.g. T_a or some input variables that are highly correlated, e.g. $m_f, T_{g,in}$ and C_{NO_x} , due to a particular engine operating state. Nevertheless, the function of an aftertreatment system mostly depends on $T_{\rm g,in}$ and $m_{\rm f}$, whose correlation is minimal from all given examples.

The operating point inlet gas temperatures are put at 150 °C, 225 °C and 300 °C according to the Table 5.3. The temperatures represent cold, warm and hot conditions in the case of a currently tuned Oxidation catalyst³. The operating points of mass flow values are following: 20 g/s, 40 g/s and 80 g/s for low, medium and high engine load.

$T_{\mathbf{g},\mathbf{in}} \mid m_{\mathbf{f}}$	Α	В	С
1	150 °C 20 g/s	150 °C 40 g/s	150 °C 80 g/s
2	225 °C 20 g/s	225 °C 40 g/s	225 °C 80 g/s
3	300 °C 20 g/s	300 °C 40 g/s	300 °C 80 g/s

Table 5.3: Oxidation catalyst operating points

The transient responses of $T_{\rm g,in}$, $C_{\rm NO}$ and $C_{\rm NO_2}$ are simulated with step deviation $\pm 10\%$ from default OP values. Clearly, the $m_{\rm f}$ can fluctuate from zero to maximum value the engine offers in a very short time as the driver steps on the gas pedal, thus a larger $\pm 25\%$ deviation has been adopted in this case. The $T_{\rm a}$ deviation is chosen to be 26.85 °C with step down to 0 °C and -26.85 °C, which simulate different seasons.

Simulations in operating points 1A, 2B and 3C provided the most distinct results, as it is shown in figures below. The comparison of catalyst transient behavior in selected operating points with other operating points is also included.

In terms of acquired data presentation, the different $m_{\rm f}$ values are displayed by distinct line styles: for $m_{\rm f} = 20$ g/s the lines are dotted, for $m_{\rm f} = 40$ g/s the lines are dashed and for $m_{\rm f} = 80$ g/s the lines are solid. This 'line code' is followed in the rest of this subsection.

There are transient responses for temperatures $T_{g,out}$, $T_{m,out}$, $T_{h,out}$ and NO_x ratios in operating points 1A, B and C for various m_f shown in Figure 5.20. The given figure shows that the higher the m_f values are, the faster are the transient responses of outlet temperatures to inlet exhaust gas temperature deviation, due to more heat transferred through incoming gas. Also, increase in m_f results in a visual decrease in NO conversion. This is understandable, because the higher the m_f the more the NO_x flows through the device, although only a limited amount of it can be converted under the given conditions. Note that the temperatures of operating points 1A, B and C are too low for the NO_x reduction, even $\pm 10\%$ $T_{g,in}$ deviations do not have significant impact on NO_x ratios.

³More parameter adjustment is required to coordinate function of OC and SCR


Figure 5.20: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$ and NO_x in OPs 1A, 1B and 1C for $T_{\rm g,in}$ deviation, ($m_{\rm f} = 20$ g/s - dotted, $m_{\rm f} = 40$ g/s - dashed and $m_{\rm f} = 80$ g/s - solid)



Figure 5.21: Transient response of $T_{\rm g,out}$, $T_{\rm h,out}$, $T_{\rm h,out}$ and $\rm NO_x$ ratios in OP 1A for $m_{\rm f}$ deviation

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Figure 5.21 depicts the influence of $m_{\rm f}$ deviation on NO_x ratios and on outlet temperatures in operating point 1A. There are very fast step changes in NO_x ratios observable in the given figure. An increase in mass flow relatively decreases the NO conversion because of a higher absolute amount of NO_x. This is in accordance with the observation in Figure 5.20. Note that the outlet temperatures are not affected by $m_{\rm f}$ deviations, since the $m_{\rm f}$ affects only the rate of catalyst heat up but not the steady state temperature values.

Figure 5.22 represents the influence of $T_{\rm a}$ deviation on outlet temperatures and on NO_x ratios in operating points 1A, 1B and 1C. The perturbations of $T_{\rm a}$ have observable influence only on the outlet temperature of the catalyst housing. The intra-catalyst temperatures are affected minimally due to a relatively small value of $k_{\rm m\to h}^4$.



Figure 5.22: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$ and NO_x ratios in OPs 1A, 1B & 1C for $T_{\rm a}$ deviation, ($m_{\rm f} = 20$ g/s - dotted, $m_{\rm f} = 40$ g/s - dashed and $m_{\rm f} = 80$ g/s - solid)

The NO_x ratios transient responses on C_{NO} deviations in operating point 1A are shown in Figure 5.23. The C_{NO} step deviations cause the fast response of NO_x ratios. The increase in C_{NO} understandably results in a rise in NO ratio and a drop in NO_2 ratio.

 $^{{}^{4}}k_{\rm m \to h} = 45 \ {\rm W}/({\rm m}^{2} \ {\rm K}^{1})$

Apparently the deviations of NO_2 have a crossover effect on corresponding NO_x ratios, hence an appropriate figure for NO_2 is not necessary, as the content of NO_2 is much smaller than the content of NO. The engine outlet NO_x concentrations can be limitedly affected by engine measures, including the EGR, thus their usage for control purposes has to be taken into account. However intra-engine means for precise NO_x concentration control have yet to be developed.



Figure 5.23: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$ and NO_x in OP 1A for $C_{\rm NO}$ deviation

There are outlet temperatures transient responses for $T_{g,in}$ step deviation in operating points 2A, 2B and 2C shown in Figure 5.24. Note that the inlet gas temperature of operating points 2x is located very close to the optimal NO conversion point. This is observable in the NO_x ratios Subfigure. Another fact worthy of attention is that the negative $T_{g,in}$ deviation from the default value has greater impact on the NO_x ratios than the positive $T_{g,in}$ deviation. This is caused by the uneven temperature dependence of the conversion reaction. Also the effect of various m_f on both the outlet temperatures and NO_x ratios is well visible in Figure 5.24. The reason of this phenomena is the same as explained in the figures above. From control point of view, the m_f has to be treated as a disturbance instead of a control variable. The m_f can not be controlled by an ECU unit, since it is controlled mostly by a driver through actual engine load.



Figure 5.24: Transient response of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$ and NO_x in OPs 2A, 2B and 2C for $T_{g,in}$ deviation, ($m_f = 20 \text{ g/s} - \text{dotted}$, $m_f = 40 \text{ g/s} - \text{dashed}$ and $m_f = 80 \text{ g/s} - \text{solid}$)



Figure 5.25: Transient response of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$ and NO_x in OPs 3A, 3B and 3C for $T_{g,in}$ deviation, (line code as in 5.24)

A similar situation as in Figure 5.24 is depicted in Figure 5.25, where outlet temperatures transient responses for $T_{\rm g,in}$ deviation in operating points 3A, 3B and 3C is shown. The first thing to notice is that the $T_{\rm g,in}$ is clearly beyond the optimal NO conversion point, since the NO₂/NO_x ratio is greater than the NO/NO_x ratio. The unevenness of the temperature influence on NO_x ratios is observable, as well as the influence of various $m_{\rm f}$ values on the NO_x ratios.

5.2 Intermediate Piping

An intermediate piping interconnects the Oxidation catalyst and the SCR catalyst and also contains the Urea injection system. Concerning the NO_x reduction, the intermediate piping does not contribute to the overall aftertreatment performance. However, from the point of view of control, this subsystem contains the main action variable of the aftertreatment system - the $C_{\rm U}$ produced from the injected urea-water solution vaporization. Therefore is desirable to study $C_{\rm U}/m_{\rm US,i}$ dependence.

A static characteristic of $C_{\rm U}$ dependence on $m_{\rm US,i}$ for $m_{\rm f} = 40$ g/s and $T_{\rm g} = 300$ °C is shown in Figure 5.26. The characteristic is linear with a slope of 3150 mol/m³ per injected gram of urea solution. This amount suffices for later reduction of nearly twice the amount of NO_x in the SCR. However, such high NO_x concentrations are well beyond engine NO_x output possibilities.



Figure 5.26: Dependence of static characteristic of $C_{\rm U}$ on $m_{\rm US,i}$

The urea-water solution has to be entirely vaporized in the intermediate piping. This process consumes a certain amount of heat from inlet gas. The corresponding temperature

transient response characteristic for discretely increasing amounts of injected urea-water solution is depicted in Figure 5.27. As can be observed from the given figure, the urea injection, in tenths of gram per second, has negligible influence on the temperature of the outlet exhaust gas. For instance, the step in urea injection from 0.1 g/s to 0.5 g/s causes a drop in outlet exhaust gas temperature of 0.2 °C.



Figure 5.27: Influence of $m_{\rm US,i}$ on outlet temperatures $T_{\rm g}$ and $T_{\rm p}$

The intermediate piping submodel contains very fast gas temperature dynamics, as can be seen in Figure 5.28. It depicts a comparison of IP submodels with (subscript B) and without (subscript A) included fast dynamics. Apparently such fast dynamic has negligible influence on the behavior of the whole submodel, therefore in can be neglected without severely compromising model fidelity. Moreover, such simplification eventually leads to about a 1.7% simulation time savings. This amount seems small, however for a more complex model the time savings will be significant.



Figure 5.28: Effect of neglected fast dynamics of IP submodel on accuracy and simulation time

5.3 SCR Catalyst

Finally, the last and the most important submodel to be validated is the SCR catalyst. The SCR catalyst utilizes the equations given in chapter 4 and its implementation is based, as the OC, on Level-2 M-File S-Function in MATLAB. Therefore, despite somewhat different catalyst parameter values and time constants, it can be assumed that the SCR possesses the same temperature behavior as the OC. Hence the findings presented in section 5.1 are also applicable, to some extent, to the SCR catalyst. The only significant difference between SCR and OC lie in implemented chemical reactions, which are connected with a different function of the device.

Unlike the OC, the SCR provides the main NO_x mitigation function of aftertreatment system, which can be quantified as a NO_x reduction efficiency ratio η . The η is defined as the amount of NO_x that has been reduced by NH_3 on the SCR catalyst outlet compared to the total NO_x amount in the catalyst inlet. The value of η is highly dependent on temperature as well as is the NH_3 loading in the catalyst. Those temperature dependencies are based on chemical reactions and corresponding rate equations, as in case of OC. However, the temperature dependencies are different from the NO_x ratios of OC because of different chemical reactions. In addition to the η , the outlet NH_3 concentration, the so called NH_3 slip, also participates in the SCR catalyst efficiency definition, because it is constrained by legislation. Thus this section is focused on study of temperature and catalyst parameter influence on η and NH_3 slip value on the outlet of the SCR catalyst.

The input parameters of the SCR are given in Table 5.4. Note that the parameters are set constant for tests in 5.3.1 and 5.3.2. Transient characteristics of these parameters are studied in 5.3.3.

Input parameter	Value	Input parameter	Value
Concentration of O_2	7000 ppm	Mass flow rate	0.04 kg/s
Concentration of NO	330 ppm	Ambient temperature	$26.85~^\circ\mathrm{C}$
Concentration of NO_2	330 ppm	Exhaust gas pressure	101 kPa
Concentration of Urea	330 ppm		

Table 5.4: SCR catalyst input parameters

The input parameter values differ from those given in 5.1. This represents exhaust gas conditions right at the SCR catalyst inlet, thus the influence of OC and IP is, in simplified way, taken into account. The inlet NO_x mixture is set at 1:1. The urea concentration

after its decomposition is considered to be exactly the stoichiometric amount of NH_3 in point of view of reaction 4.20.

5.3.1 Basic Static Characteristic

The basic static characteristic of the SCR includes only the NO_x reduction efficiency η because thermal static characteristics are virtually the same as the corresponding OC static characteristics. The main difference lies in the distinct time constants due to different catalyst dimensions.



Figure 5.29: Dependence of static characteristic of η and of $\rm NH_3$ slip on $$T_{\rm g,in}$$

The dependence of the static characteristic of η and of NH₃ slip on inlet exhaust gas temperature $T_{g,in}$ is shown in Figure 5.29. The values of η and NH₃ slip on the left hand side of given figure corresponds to the steady state of cold SCR. Almost all produced NH₃ leaves the SCR catalyst to the atmosphere and none of the NO_x content in the exhaust gas is reduced. The cold conditions with little or no NO_x reduction can be determined up to the temperature of 200 °C. Furthermore, as the $T_{g,in}$ rises over 200 °C, the η rises as well. Contrarily the NH₃ slip drops as more NH₃ is exploited for the NO_x reduction reaction. The η reaches its maximum of 0.91, 91% respectively, at a temperature of close to 350 °C, and the NH₃ slip is 14.76 ppm, which is well below 25 ppm regulatory limits [33]. When the $T_{g,in}$ rises to over 360 °C, the NH₃ oxidization gains significance. Consequently, it results in a lack of NH₃ for the NO_x reduction, and thus the η drops.

The maximal value of η under the given conditions could be even higher if more Urea is injected in such manner, so that all participating chemical reactions have stoichiometric amounts of NH₃.

5.3.2 Effect of Catalyst Parameters on Selected Static Characteristics

The SCR catalyst parameters used are given in Table 5.5. The rest of the parameters are the same as in the case of the Oxidation catalyst, and can be found in Table 5.2, since it is anticipated that the monolith and housing of the SCR catalyst are made from identical materials as are the monolith and housing of the OC.

Parameter	Value	Parameter	Value
# of SCR cells	10	Cell length	0.01 m
SCR housing outer diam.	$0.37 \mathrm{~m}$	Catalyst length	0.1 m
Active cat. surf. area	$19200 \text{ m}^2/\text{m}^3$	Void fraction	0.6836
Channel hydraulic diam.	$0.0018 {\rm m}$	Reaction site density	0.080 mol/m^2

Table 5.5: SCR catalyst physical parameters

The design of the experiment is very similar to the experiment noted in subsection 5.1.2. The simulations for every parameter value are carried out with increasing value of $T_{\rm g,in}$ ranging from 100 °C to 460 °C with a step of 20 °C. The studied parameter is for every simulation set from 70% to 130% of its default value as given in Table 5.5, with a step of 15%. The ±30% parameter range covers various SCR catalyst configurations. The number of SCR catalyst cells $n_{\rm SCR}$ is an exception, because its values belong to particular value set⁵.

The line code is used the same as in 5.1.2, where particular parameter values are distinguished by different line widths in corresponding figures. The wider the displayed line is, the higher the studied parameter value will be.

As was noted before, the SCR catalyst submodel has utilized the same temperature mechanism as the OC submodel. Therefore, temperature static characteristics and temperature transient response characteristic have a similar shape to those presented in 5.1, except for the time scale. Different time scale is understandable because of larger SCR catalyst volume and thus higher time constants. Therefore, the mentioned characteristics are not presented in this subsection. The η is distinct from the NO_x ratios of OC, thus corresponding static characteristics are presented in the following figures.

First of all, a dependence of the static characteristic of NO_x reduction efficiency η and of NH₃ slip on $T_{g,in}$ and n_{SCR} is shown in Figure 5.30. A SCR submodel order, determined

 $^{{}^{5}}n_{\rm SCR} \in \{1, 2, 3, 4, 6, 10\}$ with default value $n_{\rm SCR, def} = 10$

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by the value of $n_{\rm SCR}$, highly affects the completeness of NO_x reduction. The higher the $n_{\rm SCR}$ is, the higher the η and the maximal NO_x reduction point will be shifted slightly to the region of lower temperatures. The distance between lines for rising $n_{\rm SCR}$ values decreases, therefore is not desirable to choose too high a $n_{\rm SCR}$ because of decreasing influence on accuracy improvement and also because of increased simulation time. Therefore a compromise between the $n_{\rm SCR}$ value and the model accuracy have to be chosen, especially for real time control. Note that the length of the catalyst is constant, thus for increasing $n_{\rm SCR}$ the single cell length decreases.



Figure 5.30: Dependence of static characteristic of η and of NH₃ slip on $T_{\rm g,in}$ and $n_{\rm SCR}$, $(n_{\rm SCR} \in \{1, 2, 3, 4, 6, 10\}, n_{\rm SCR, def} = 10)$

The NO_x reduction efficiency is highly dependent on catalyst dimensions. The $d_{\rm h,SCR}$ and $x_{\rm SCR}$ influence on NO_x reduction efficiency η and NH₃ slip are shown in Figures 5.31 and 5.32



Figure 5.31: Dependence of static characteristic of η and of $\rm NH_3$ slip on $T_{\rm g,in}$ and $d_{\rm h,SCR}$



Figure 5.32: Dependence of static characteristic of η and of $\rm NH_3$ slip on $T_{\rm g,in}$ and $x_{\rm SCR}$

As expected, the bigger the catalyst is, the higher the η will be. The influence of the catalyst housing diameter $d_{h,SCR}$ on η is considerably higher than the catalyst cell length x_{SCR} due to a higher volume increment per unit increase in parameter. However, catalyst volume also has to be constrained due to onboard volume and price issues. Moreover, a bigger catalyst tends to have longer heating up phases, thus it experiences longer periods of cold operating conditions. Therefore, a proper compromise between catalyst volume, price, desired η and NH₃ slip has to be determined independently from case to case.



Figure 5.33: Static char. of η and of NH₃ slip for varying $T_{\rm g,in}$ and ε

Figure 5.33 depicts the dependence of the static characteristic of NO_x reduction efficiency η and of NH_3 slip on $T_{g,in}$. As in case of the OC, the rise in ε decreases the η . This is caused by dilution of reaction site density due to more catalyst monolith volume beeing accessible to the exhaust gas, while the $L_{Pt,SCR}$ is constant. Under that condition it is less probable that NO_x will come across the reaction site, thus it results in lowered

 η and increased NH₃ slip at the given temperature. However, altering the ε of monolith is limited due to physical limits of material engineering.

There is a dependence of the static characteristic of NO_x reduction efficiency η and of NH_3 slip on $T_{g,in}$ and G_{cat} , as depicted in Figure 5.34. This catalyst monolith property has proportional influence on η , as expected. The higher the G_{cat} value is , the higher the resulting η will be due to more NO_x being reduced over a larger active catalyst area.



Figure 5.34: Static char. of η and of NH₃ slip for varying $T_{g,in}$ and G_{cat}

Figure 5.35 displays the influence of $L_{\rm Pt,SCR}$, the SCR monolith washcoat property, on NO_x reduction efficiency η and NH₃ slip. Any significant influence of this parameter is observable in the given figure. Unlike in the OC, the SCR catalyst $L_{\rm Pt,SCR}$ determines the rate of ammonia surface coverage generation as seen in equation 4.10. Therefore, rather than steady state values of η , the ammonia surface coverage $\theta_{\rm NH_3}$ is affected.



Figure 5.35: Static char. of η and of NH₃ slip for varying $T_{g,in}$ and $L_{Pt,SCR}$

5.3.3 Transient Response Characteristics

The inlet gas temperature step from 30 °C to 340 °C at time 0 s has been used for the transient response characteristics simulation. Because the thermal behavior is similar to the OC, only η and NH₃ slip transient responses for ±30% parameter changes are studied in this subsection.

5.3.3.1 NO_x Reduction Efficiency Transient Responses

Several of the most significant NO_x reduction efficiency and ammonia slip transient response characteristics are presented in the following figures. The remaining figures for transient characteristics can be found on the attached CD.

Figure 5.36 depicts the transient response of NO_x reduction efficiency η and of NH₃ slip for various $n_{\rm SCR}$. The higher the $n_{\rm SCR}$ value is, the faster will be the η and NH₃ slip transient response with higher steady state values, which is in agreement with the findings in the previous subsection. Higher $n_{\rm SCR}$ provides a more precise computation, therefore higher η can be obtained. The difference between steady state values of η are 16.2%, 6.6%, 3.7%, 2.3% and 1% for $n_{\rm SCR} = 1, 2, 3, 4$ and 6 respectively in comparison with $n_{\rm SCR,def} = 10$.



Figure 5.36: Transient response of η and of NH₃ slip for various n_{SCR} , $(n_{\text{SCR}} \in \{1, 2, 3, 4, 6, 10\}, n_{\text{SCR}, \text{def}} = 10)$

The transient response of NO_x reduction efficiency η and of NH_3 slip for various $d_{h,SCR}$ is shown in Figure 5.37. The higher the $d_{h,SCR}$ is, the higher will be the values of η that can be reached. However, it is redeemed by a slower rise time due to slower catalyst warm up, since a larger catalyst takes more time to reach particular temperature than does a smaller one. A similar effect can be seen for the x_{SCR} parameter. Nevertheless,

the amplitude of that effect is lesser than the effect of $d_{h,SCR}$ due to a smaller volume increment.



Figure 5.37: Transient response of η and of NH₃ slip for various $d_{\rm h,SCR}$

As a last example of parameter influence on SCR catalyst transient response of NO_x reduction efficiency and of NH_3 is chosen the void fraction ε is chosen, as seen in Figure 5.38. The higher ε is, the faster the rise time of η will be due to faster catalyst warm-up caused by more intense heat transfer. However, higher ε results in lower steady state values of η . This is connected mainly with reaction site dilution.



Figure 5.38: Transient response of η and of NH₃ slip for various ε

Findings presented in this subsection provide information about how the changes of a particular parameter affect the catalyst dynamic behavior. This information is helpful when a designed control strategy has to take into account the effects of catalyst aging.

5.3.3.2 Input Variable Transient Responses

A few temperature and NO_x reduction efficiency transient responses of SCR catalyst to step change of input variables in selected operating points, as seen in Table 5.4, are studied in this subsection.

There is a single input variable step change introduced in every simulation. The remaining input variables are left unchanged. This arrangement allows for the influence of individual input variables on catalyst transient behavior to be observed. Likewise, in the case of an OC, the remaining SCR catalyst parameters from Table 5.5 are left at their default values.

The selected operating points (OPs) are given in Table 5.6. Operating points are defined analogically to the CO operating points by particular values of $T_{\rm g,in}$ and $m_{\rm f}$. The operating point inlet gas temperatures are put at 240 °C, 300 °C and 340 °C according to Figure 5.29. The temperatures represent cold, warm and hot conditions in the case of currently tuned SCR catalyst⁶. The operating points mass flow values are selected the same for an OC: 20 g/s, 40 g/s and 80 g/s for low, medium and high engine load.

$T_{\mathbf{g},\mathbf{in}} \mid m_{\mathbf{f}}$	Α	В	С
1	240 °C 20 g/s	240 °C 40 g/s	240 °C 80 g/s
2	300 °C 20 g/s	300 °C $40 g/s$	300 °C 80 g/s
3	340 °C 20 g/s	340 °C 40 g/s	340 °C 80 g/s

Table 5.6: SCR catalyst operating points

The transient responses of $T_{\rm g,in}$, $C_{\rm NO}$, $C_{\rm NO_2}$ and $C_{\rm U}$ are simulated for step deviation $\pm 10\%$ from default or for default operating point values. The $m_{\rm f}$ can fluctuate from zero to maximum value in a very short time, therefore to take this fact into account, a larger $\pm 25\%$ deviation has been addopted. The $T_{\rm a}$ deviation is 26.85 °C with step down to 0 °C and -26.85 °C, which simulate the different seasons.

The simulation for all nine operating points has been carried out. The most distinct results are presented in the following figures. The data presentation method used is the same as in subsection 5.1.3.3.

Figure 5.39 depicts the transient responses of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$, η and NH₃ slip in operating points 1A, 1B and 1C for $T_{g,in}$ deviation. The apparent similarity to the corresponding OC transient response is noticeable, however the time constant of thermal

⁶More parameter adjustment is required to coordinate function of OC and SCR

behavior for a SCR catalyst is nearly four times slower than the time constant for an OC for all given mass flow conditions. The inlet gas temperature step results in a slight increase in η and a decrease in NH₃ slip. Nevertheless, the temperature is too low for a significant NO_x reduction to take place. The temperature transient response is faster because more heat is transported with increasing mass flow values. Contrarily, the η is lower because of more NO_x to be converted in constant time flows through the catalyst.



Figure 5.39: Transient response of $T_{\rm g,out}$, $T_{\rm n,out}$, $T_{\rm h,out}$, η and NH₃ slip in OPs 1A, 1B and 1C for $T_{\rm g,in}$ deviation, ($m_{\rm f} = 20$ g/s - dotted, $m_{\rm f} = 40$ g/s - dashed and $m_{\rm f} = 80$ g/s - solid)

From Figure 5.40, which shows the transient response of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$, η and NH₃ slip in OP 1A for m_f deviation, it is clearly observable, that outlet temperatures are not affected by mass flow steps. Unlike the temperatures, the η and NH₃ are susceptible to mass flow disturbances. The actual cause can be found in increased residence time, which is favorable for better NO_x reduction.

From previous observations, it can be deduced that the SCR catalyst transient response characteristic of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$, η , and NH₃ slip for T_a deviation is similar to corresponding transient characteristics of the OC catalyst. However, the higher time constant value makes the transient response comparatively slower.



Figure 5.40: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$, η and NH₃ slip in OP 1A for $m_{\rm f}$ deviation



Figure 5.41: Transient response of $T_{\rm g,out}$, $T_{\rm h,out}$, η and NH₃ slip in OP 1A for $C_{\rm NO}$ deviation

Figure 5.41 shows the influence of $C_{\rm NO}$ step on outlet temperatures, NO_x reduction efficiency and ammonia slip in operating point 1A. Only small peaks in time of $C_{\rm NO}$ steps of are observable. This is caused by the relatively low temperature of inlet gas and also by low mass flow. The more noticeable influence of $C_{\rm NO}$ deviation is expected for higher values of both mentioned input variables.

The influence of $C_{\rm U}$ deviation especially on η and NH₃ slip in operating point 1A is depicted in Figure 5.42. The strong direct correlation between NH₃ slip and $C_{\rm U}$ is visible in given figure. Spare ammonia generated from urea decomposition is released directly into the atmosphere. The low temperature dampers the chemical reactions of the NO_x reduction, thus only slight changes in η values are visible.



Figure 5.42: Transient response of $T_{\rm g,out}$, $T_{\rm n,out}$, η and $\rm NH_3$ slip in OP 1A for $C_{\rm U}$ deviation



Figure 5.43: Details of transient responses of η and NH₃ slip in OP 1A for $C_{\rm U}$, $m_{\rm f}$ and $C_{\rm NO}$ deviation

Figure 5.43 depicts magnified parts of η and NH₃ slip transient characteristics for $C_{\rm U}$, $m_{\rm f}$ and $C_{\rm NO}$ deviation. Concerning the speed of exhaust gas flowing through the device, the displayed transient responses are naturally fast processes. A slight delay is visible for the NH₃ slip for both $C_{\rm U}$ and $m_{\rm f}$ deviations. The η is most distinctly affected by $C_{\rm NO}$ deviation, where a non-minimum phase of η results in a negative peak.

A transient response of $T_{g,out}$, $T_{m,out}$, $T_{h,out}$, η and NH₃ slip in operating point 2A, 2B and 2C for $T_{g,in}$ deviation is shown in Figure 5.44. The inlet exhaust gas temperature step deviations under the warmed catalyst condition result in significant changes in η and in correlated NH₃ slip. Moreover, an uneven η behavior toward increasing temperature is visible for the step up of $T_{g,in}$ at time 500 s. Essentially, the mass flow has a non-negligible impact on η . Note that for $m_f = 20$ g/s the η exceeds the 90% line, which is slightly more than 84% in the case of medium m_f and substantially more than the nearly 64% for low m_f . Apparently, the lower the mass flow is, the more complete the NO_x reduction can take place due to the lower space velocities and thus due to higher residence time. However this dependence is not proportional.



Figure 5.44: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$, η and NH₃ slip in OPs 2A, 2B and 2C for $T_{\rm g,in}$ deviation, ($m_{\rm f} = 20$ g/s - dotted, $m_{\rm f} = 40$ g/s - dashed and $m_{\rm f} = 80$ g/s - solid)

Finally, Figure 5.45 shows the transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$, η and NH₃ slip in operating points 3A, 3B and 3C for $T_{\rm g,in}$ deviation. Interestingly, for $m_{\rm f} = 80$ g/s a 10% step up of $T_{\rm g,in}$ at time 500 s results in an η increase of about 16.5% of pre-step value,

however a 20% step down of $T_{g,in}$ at time 1000 s results in a 61% η decline compared to pre-step value. Clearly, the temperature uneveness has an opposite impact for higher temperatures, unlike taht for the lower to medium temperatures. However, this finding applies only for high mass flows. The lower mass flow conditions are not so susceptible to inlet exhaust gas temperature deviations. The apparent cause can be found in the ammount of heat carried by the exhaust gas.



Figure 5.45: Transient response of $T_{\rm g,out}$, $T_{\rm m,out}$, $T_{\rm h,out}$, η and NH₃ slip in OPs 3A, 3B and 3C for $T_{\rm g,in}$ deviation, ($m_{\rm f} = 20$ g/s - dotted, $m_{\rm f} = 40$ g/s - dashed and $m_{\rm f} = 80$ g/s - solid)

Chapter 6

SCR System Control

A particular demonstration of aftertreatment system control strategy utilizing a single PID controller is presented in this section. First, the overall control strategy is described. Next, the aftertreatment system parameters adjustment takes place so that the whole model can be simulated afterward in series with the diesel engine model provided by the Honeywell company. Further, an optimal urea injection map for the given operating points is acquired using the outlet exhaust gas conditions of the given diesel engine model as an exhaust gas aftertreatment system input data. Finally, a PID controller with composite control error is used to control the complete aftertreatment system model. Discussion of simulation results follows afterward.

6.1 Control Strategy

The efficiency of the whole exhaust gas system aftertreatment depends firstly on wellmastered physical design of the device itself, secondly on proper diesel engine calibration, and finally on a properly designed control strategy. The control strategy has to regard several criteria such as NO_x reduction efficiency, fuel consumption, urea consumption and more. However the control strategy influence should not be overestimated. Naturally, the selection of any control strategy cannot turn a weakly designed exhaust gas aftertreatment system into a device with cutting edge efficiency.

A primary purpose of an exhaust gas aftertreatment system control strategy is to provide NO_x reference tracking, physical design inaccuracies mitigation and minimization of disturbance influence propagation while ensuring that the NH_3 is kept safely under limit given by legislation. A feedback control in combination with a commonly used feedforward control, which utilizes the engine operation data maps, seems to be a suitable solution for the presented control strategy objectives. The feedback control can be utilized with the following configurations:

- An MPC controller for the engine and the AT system, which are treated as a compact unit. The engine is controlled in such a way to provide the optimal operating conditions for the AT system in all engine operating points, while respecting the fundamental engine operation restrictions, e.g. intake manifold pressure, airto-fuel ratio, etc. Interested readers can find further details about MPC usage for automotive applications in [34].
- A cascade of PID controllers, where the setpoints for the engine controlling PIDs are computed as the output of PIDs controlling the NO_x reduction and NH₃ slip of the exhaust gas aftertreatment system. The engine setpoints determined in a such manner would provide favorable operating conditions for AT system.

Clearly, the MPC controller is able to provide superior performance, due to more information implemented in control. Nevertheless, for demonstration purposes, a simplified version of a PID-based deviation control strategy is implemented in this thesis. A possible solution for aftertreatment system control is depicted in Figure 6.1



Figure 6.1: Aftertreatment system control schematic

The control strategy takes into account the need for maximizing the η , while keeping the NH₃ slip¹ under given regulatory limits. A single PID controller is used for control.

¹Further denoted as $NH_{3,d}$

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The only controlled input is $m_{\text{US},i}$, with implemented saturation to provide anti-windup functionality. The observable outputs are $\text{NO}_{x,\text{out}}$, $\text{NH}_{3,\text{d}}$ and $T_{\text{g,out}}$, since corresponding sensors are available in the market. The composite control error e consists of partial control errors e_1 , e_2 and NO_x reference. The e_1 represents a difference between the $\text{NO}_{x,\text{d}}$ value and the optimal $\text{NO}_{x,\text{d}}^*$ value. Likewise, the e_2 denotes a restriction of NH_3 slip, where $f(\text{NH}_{3\,\text{d}}) = \min(0, \text{NH}_{3,\text{d}}^* - \text{NH}_{3,\text{d}})$. The composite control error e can be therefore expressed by the following equation:

$$e = \varphi(\underbrace{\mathrm{NO}_{\mathrm{x,d}} - \mathrm{NO}_{\mathrm{x,d}}^*}_{e_1} - \underbrace{\Delta\mathrm{NO}_{\mathrm{x,ref}}}_{\mathrm{ref}}) + \underbrace{\rho\min\left(0, \mathrm{NH}_{3,\mathrm{d}}^* - \mathrm{NH}_{3,\mathrm{d}}\right)}_{e_2}$$
(6.1)

where $\frac{\rho}{\varphi}$ stands for the weight factor, which determines the significance of η and NH_{3,d}. Clearly such a composite control error results in a compromise between optimal NH_{3,d} and η for the given operating point, therefore the given performance parameters will be suboptimal depending on the weight factor value.

The ammonia slip restriction of the presented control strategy exploits the softconstrain limitation due to usage of aggregate control error. However, the hard-constrain limitation of $NH_{3,d}$ would be more appropriate.

6.1.1 Basic Data of the Diesel Engine Model

The mean value model of a given heavy trucking diesel engine is based on real engine data measurement and it is provided by the Honeywell company. The $m_{\rm f}$, $T_{e,out}$ and NO_x characteristics of this engine model are presented in this section. These data are key to successful aftertreatment system model adjustment, since all three mentioned variables are considered as the main inputs of an aftertreatment system.

As it is shown in Figure 6.2(a), the diesel engine model has 36 defined steady state operating points for various fuel injection quantities (IQ) and engine speeds (N_{eng}) . The operating points are evenly distributed across the whole operating range of the given engine from idle to heavy load operating conditions.

Corresponding mass flows are depicted in Figure 6.2(b). Note that the mass flow values are ten times greater than mass flow used for model validation in the previous chapter. Therefore the aftertreatment system dimensions have to be altered to work properly in series with this engine.



Figure 6.2: Engine model data set 1

Other important engine characteristics, from the aftertreatment system point of view, are the engine out exhaust gas temperatures (measured downstream of the engine turbine) depicted in Figure 6.3(a) and the engine out NO_x concentrations shown in Figure 6.3(b). The outlet temperatures vary from about 240 °C to 600 °C, which overlaps the minimum and maximum operating temperatures of the SCR catalyst. However, the diesel engine used contains an EGR system. Therefore, the EGR-SCR cooperation will provide sufficient NO_x mitigation, which would likely cover the majority of engine operating conditions.



Figure 6.3: Engine model data set 2

Engine out NO_x emissions are significant especially under high IQ and low engine speed with noticeable decrease toward high engine speed, where the EGR starts working.

The region of excessive NO_x engine out emissions is an area of major interest for applying the SCR reduction capability. According to the SCR function, the only problem with NO_x reduction will be caused by operating point 6, due to low exhaust gas temperature that is almost 10 °C below the minimal operating temperature of the SCR catalyst.

6.1.2 Fitting of the Aftertreatment System Model

Since the engine model possesses higher mass flow than was used for the model validation, the aftertreatment model parameters have to be altered. The parameters that are especially suitable for adjustment are the dimensions and pmg loadings of both catalysts, because these parameters have the greatest effect on the desired NO_x conversion/reduction. Except for material selection, these parameters are the first choice for catalyst manufacturers.

The exhaust gas aftertreatment parameter fitting has been carried out in an iterative manner, while seeking higher desired NO_x reduction efficiency and lower NH_3 slip as given operating conditions defined by operating point data. A complete overview of the altered parameters for both catalysts is given in Table 6.1.

OC			
# of OC cells	4	Cell length	0.02 m
OC housing outer diam.	$0.15 \mathrm{~m}$	Catalyst length	0.08 m
Active cat. surf. area	$3369~\mathrm{m^2/m^3}$	Reaction site density	0.021 mol/m^2
SCR			
# of SCR cells	10	Cell length	0.04 m
SCR housing outer diam.	0.40 m	Catalyst length	0.4 m

Table 6.1: OC and SCR catalysts parameter adjustment

For the Oxidation catalyst it was necessary to adjust, besides the dimensions, the monolith properties such as G_{cat} , since the optimal NO_x conversion point has to be shifted closer to the region of higher temperatures, than simple dimension adjustment allowed. The number of cells of the Oxidation catalyst was decreased from 10 to 4, which was recognized as satisfactory for sufficiently accurate results to be obtained from simulations. The situation in the case of SCR catalyst was simpler: dimension adjustment was sufficient to allow the SCR catalyst to handle a high mass flow operation. The need

for more accurate results lead to usage of full 10 cells per SCR catalyst. Note that no parameter was changed in case of the intermediate piping.

The following figures show the properties of fitted aftertreatment system in all engine operating points. Figure 6.4 depicts NO_x ratios of the adjusted Oxidation catalyst. The NO/NO_x ratio, shown in Figure 6.4(a), has values around 0.5 for the region of low engine rpms, where the major SCR working area is anticipated. However, the NO/NO_x ratio drops significantly for high temperature conditions in the area over 1500 rmps and over 150 mg/stroke of fuel injection quantity (the corresponding rise of NO_2/NO_x ratio can be seen in Figure 6.4(b)). Nevertheless, the temperature constrains the SCR function in this region, therefore it is not an issue.



Figure 6.4: Properties of adjusted OC

Using various engine operating point data as input for an aftertreatment system model, it was necessary to determine the dependence of urea concentration on engine speed and fuel IQ. This is depicted in Figure 6.5(a). The $C_{\rm U}$ obtained per gram of injected urea solution is decreasing with increasing exhaust gas temperature and mass flow, due to the constant amount of urea dispersed in larger exhaust gas volume. Also, a thermal expansion of exhaust gas contributes to this process.

Knowledge of the $C_{\rm U}$ static characteristic is crucial to ensure that proper $C_{\rm U}$ value is achieved at a particular operating point. The close-to-optimal $C_{\rm U}$ determined for the SCR catalyst is shown in Figure 6.5(b). These $C_{\rm U}$ values were determined iteratively, while seeking maximal η and less than 12.5 ppm NH₃ slip, which is a half of the maximal allowed peak value.



Figure 6.5: Properties of IP



Figure 6.6: Properties of adjusted SCR, part 1

The actual urea solution injection quantity $m_{\rm US,i}$, denoted in grams of urea solution per second for all 36 engine operating points, is depicted in Figure 6.6(a). Tailpipe NO_x emissions obtained under the given urea injection conditions are shown in Figure 6.6(b).

The resulting NO_x reduction efficiency η and NH_3 slip is depicted in Figure 6.7. The maximal η is reached for operating points with a high engine NO_x output, with the exception of low temperature conditions in engine operating point 6, while the NH_3 slip is successfully held below the 12.5 ppm threshold. The displayed static characteristics of η and $NH_{3,d}$ are not smooth due to coarse grid step, which results in significant error.



Figure 6.7: Properties of adjusted SCR, part 2

Overall, the average η computed for all engine operating points is 59.7%. For engine operating points that have exhaust gas temperatures within the 260 °C to 450 °C range, the average η is 77%. Remember that the NO_x reduction efficiency of a given aftertreatment system is additional to the NO_x reduction capabilities of the EGR already installed on the engine. Depending on actual EGR performance, it is highly probable that the combined diesel engine - exhaust gasaftertreatment setup complies with the EURO VI emission regulation. Note that the operating temperature range of the current aftertreatment model is narrower than the temperature operating range given in chapter 2. This depends on the aftertreatment system model fitting. Therefore, when more optimization effort is applied, an even higher η is likely to be reached.

6.2 Simulations

A control strategy, presented in section 6.1, has been applied to a complete aftertreatment system model. Simulation of control responses was carried out for NO_x reference tracking and for step deviations of all regarded disturbance variables in diesel engine operating point no.4, where the aftertreatment system provides major NO_x reduction capability due to favorable temperature conditions.

The PID controller is iteratively tuned to provide NO_x reference tracking without any overshoot. The corresponding PID controller parameters are P = 5.8, I = 3.2 and D = 0.1. Further, gains φ and ρ are set to $\frac{1}{700}$ and $\frac{1}{40}$ respectively, and the weight factor $\frac{\rho}{\varphi}$ equals 17.5. Considering the steady state values of NO_{x,d} = 90.2 ppm and NH_{3,d} = 2.6 ppm for operating point no.4, the weight of NH_{3,d} equals 45.5, which is about half of the absolute weight of NO_{x,d}. Therefore a currently tuned controller favors higher η than lower ammonia slip.

The following figures depicts the most significant results obtained from simulations. Figure 6.8 depicts the response of the controlled AT system on 20% NO_x reference step, where a nominal $NH_{3,d}$ value equals the optimal $NO_{x,d}$ for operating point no. 4. The NO_x reference tracking has steady s state error of 2.3 ppm, which accounts for the influence of the higher than nominal $NH_{3,d}$. Almost perfect tracking is obtained for the positive 20% NO_x reference step, for which the ammonia slip is below the nominal value, thus only e_1 is applied for control. The $NH_{3,d}$ is corelated with the action variable $m_{US,i}$ as expected.



Figure 6.8: AT system control: NO_x reference tracking for OP 4 of diesel engine, 20% reference step amplitude

Figure 6.9 shows a response of the controlled AT system for the mass flow 5% step disturbance from the nominal value of the corresponding operating point. Even though the mass flow disturbance is symmetrical, its effect on the aftertreatment system response is highly asymetrical because of the ammonia slip control error e_2 restriction. The negative disturbance step is compensated for well, unlike the positive disturbance step, where the desired steady state NO_x value is not reached due to higher than nominal NH_{3 d}.



Figure 6.9: AT system control: $m_{\rm f}$ deviation for OP 4 of diesel engine, 5% deviation steps amplitude



Figure 6.10: AT system control: $T_{\rm g,u}$ deviation for OP 4 of diesel engine, 2% deviation steps amplitude

A response of a controlled aftertreatment system on engine outlet exhaust gas temperature 2% step disturbance from nominal value is shown in Figure 6.10. As can be seen, the positive temperature disturbance step is compesnsated for without problems, due to a higher than nominal ammonia consumption in a higher exhaust gas temperature environment. Unlike the positive temperature step, the negative temperature step results in a severe rise in $NO_{x,d}$, which the control system can't compensate for. Corresponding $NH_{3,d}$ is observable in the lower subfigure. This is caused by the asymmetrical sensitivity of SCR to exhaust gas temperature changes as has been observed in chapter 5. As the disturbance passes away, the system sets up on initial state values. Note that compensation peaks are related to fast exhaust gas flow dynamics.



Figure 6.11: AT system control: $N_{\rm eng}$ and IQ deviations for OP 4 of diesel engine, 5% deviation step amplitude

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The least simulation, which mimics a real-world driving cycle, is depicted in Figure 6.11. Until now, only single disturbance variable deviation has taken place in one simulation. In this case, a 5% deviations of engine speed and IQ from nominal operating point no.4 values are introduced into the complete model. Since IQ and engine speed define engine operating points, their deviation applies for all input model variables. It is possible to see from the given figure that the $NO_{x,d}$ tracks nominal/reference values precisely, while the $NH_{3,d}$ is below nominal values. Otherwise, a compromise between $NO_{x,d}$ and $NH_{3,d}$ values take place.

Chapter 7 DPF Model

This chapter briefly describes DPF modeling since a full and thorough description is out of the scope of this thesis. The major governing phenomena are outlined in accordance with the literature. Further development steps are needed to obtain a numerical model.

As was mentioned in chapter 2, the DPF could easily be damaged by the exothermic soot regeneration process, while the temperature during regeneration reaches the melting point temperature of the honeycomb substrate. The main purpose of the DPF model is therefore to provide information about soot loading and thus about the state of the DPF soot repletion. This information is crucial for prediction of soot regeneration process behavior. Consequently, it is possible to predict the amount of heat released during DPF regeneration and also temperature conditions within the DPF. With proper control of exhaust gas flow through the DPF implemented, the damage potential of DPF regeneration can be minimized.

The DPF model also provides information about the exhaust gas pollution content that is reduced during DPF regeneration phase. Therefore, incorporating the DPF model into the ECU unit leads to an improvement in exhaust gas pollution mitigation and provides an improvement of soot trap durability.

7.1 Structure of DPF Model

The DPF modeling approach is to a certain extent analogical to SCR modeling, however substantial differences exist. Also in this case the 1D model is used.

The DPF can be represented by two channels that are alternatively enclosed in op-

posite ends as it is shown in Figure 7.1. As the exhaust gas flows through the inlet channel it slows down and passes though the filter wall, while the soot is being trapped in substrate pores and on the surface of the inlet channel. The exhaust gas has properties like temperature T_x , velocity v_x , density ρ_x and pressure p_x in both channels, where lowered subscript x expresses inlet i and outlet o channels. The state of a channel wall is described by temperature T_w , velocity of gas flow through the wall v_w and wall material density ρ_w .



Figure 7.1: DPF model schematic, based on [35]

7.2 Governing Phenomena

The DPF model should contain two dominant phenomena according to the DPF function.

The first relevant phenomena to be modeled is the filter back-pressure in relation to differing operation parameters and soot loading [35]. A total pressure drop model, presented in [36], can be computed as a sum of ceramic substrate pressure drop and of soot pressure drop. This is well described by Darcy's law in [35] and [37].

The second important phenomena consists of chemical and thermal processes that take place in the filter [35]. Generally, this process occurs during soot regeneration. The soot regeneration process can be described by a set of mass, momentum and energy balance equations as well as the corresponding chemical reaction mechanism.

Chapter 8 Conclusion

Two main goals have been set for this thesis. Firstly to propose, develop and implement an exhaust gas aftertreatment model suitable for heavy-duty trucking applications, while complying EURO VI legislation; secondly to propose and implement an appropriate control strategy for a prepared aftertreatment system and to show validity of the proposed model and control strategy by simulations.

The first goal was satisfied on the basis of information obtained from thorough background research of currently used exhaust gas aftertreatment systems and technologies. Based on a detailed properties comparison of reviewed exhaust gas aftertreatment technologies, a suitable exhaust gas aftertreatment system containing an upstream Oxidation catalyst and a downstream SCR catalytic converter was chosen. Utilizing acquired information from current literature, submodels of Oxidation catalyst, intermediate piping and SCR catalyst were developed and implemented in MATLAB/Simulink. The submodels were validated through a series of tests, which also revealed the dependencies of submodel behavior on individual submodel parameter values. Validation of the SCR submodel function was carried out in operating points that mimic real-world situations. The implemented exhaust gas aftertreatment model showed good simulation results toward anticipated outcomes of a comparable realistic system.

The second goal of this thesis was accomplished by proposal and implementation of an aftertreatment system control strategy based on PID controller with aggregate control error, which takes into account both NO_x reduction efficiency and NH_3 slip by weighting factor. The implementation of the control strategy has utilized realistic diesel engine data provided by the Honeywell company. The control strategy, actually making a compromise between both antagonistic goals - maximal NO_x reduction efficiency and minimal NH_3 slip, was simulated in MATLAB/Simulink on a prepared exhaust gas aftertreatment model. Furthermore, the weighting factor of the proposed control strategy can be tuned to ensure optimal results of the aftertreatment system while the engine is undergoing an emission test cycle.

The simulations of both the control strategy and the underlying exhaust gas aftertreatment model showed good results toward accuracy and disturbance compensation within vicinity of the selected diesel engine operating point. The peak NO_x reduction efficiency of 96.7% was reached for a diesel engine operating point 3. Overall, the average NO_x reduction efficiency for all engine operating points was computed to be 59.7% and average NO_x reduction efficiency of 77% was determined for engine operating points within the exhaust gas temperature range of 260 °C to 450 °C. The exhaust gas aftertreatment model NO_x reduction efficiency is additional to the NO_x mitigation capabilities of the engine EGR, thus it is highly probable that the composed diesel engine-aftertreatment system setup will comply to strict EURO VI emissions legislation.

The obtained exhaust gas aftertreatment system model runs faster than real-time on an ordinary PC, even with uncompiled ant not optimal code. Nevertheless, it is still too much complex and demanding of computational power to be operated on automotive Engine Control Unit. Therefore, additional simplification and optimization is desirable.

Along with testbed calibration and control purposes, other possible utilizations of the obtained exhaust gas aftertreatment model can be found in investigation of the exhaust gas aftertreatment system behavior under varying operational conditions, for making predictions of the performance at these conditions and for designing new experiments for model validation. Additionally, the dependencies of catalyst behavior on the varying catalyst parameter values that have been presented in this thesis can be used in the Co-Design of the catalytic converters in manufacturing practice.

In a further work, a validation of the exhaust gas aftertreatment model on realistic data measured on the exhaust gas aftertreatment testbed will be performed. Additional work can include a substantial reduction of computational time by the implementation of the model into the programming language C or in implementation of advanced control algorithms on the model such as Extended Kalman Filter or MPC controller.
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Apendix A

Background Research

For the purpose of this thesis, a preliminary background research has been carried out. It is divided into two parts. The first part deals with a survey of available exhaust gas aftertreatment technologies and setups, to provide a broad insight into studied issues. The second part is focused on a survey of different exhaust gas aftertreatment system modelling approaches.

A.1 Exhaust gas aftertreatment technologies and setups

Collected materials, which are closely related to the studied topics, are briefly reviewed for the purpose of gaining an insight into aftertreatment technology and setup issues.

A.1.1 General Topics

1. SRC-only Concept for Heavy-duty Euro VI Applications, (2009), Article Robert Cloudt, Rik Baert, Frank Willems, Marco Vegouwe

View on possible Euro VI-compliant aftertreatment setups is given. An innovative SRC-only aftertreatment setup is proposed. The brand-new setup is compared with two other possible Euro VI aftertreatment setups. According to the results, the SRC-only setup is favored as a both emission and cost efficient solution for Euro VI NO_x and PM abatement for HD applications.

2. FreedomCAR - Aftertreatment Subsystem Development [2] (2005), Final report

Lisa A. Prentiss

Brief overview of the generally used catalysis and filtering aftertreatment technologies:

- (a) $DeNO_x$
 - Non-thermal Plasma Catalysis
 - Active Lean NO_{x} Catalyst
 - \bullet NO_{x} Adsorber
- (b) PM reduction
 - Diesel oxidation catalyst
 - Catalyzed Particulate filter (regeneration technologies described)
- (c) $DeSO_x$
 - Disposable/Off-line Regenerable
 - $\bullet~\mathrm{NO}_{\mathrm{x}}$ Adsorber Desulfation Catalyst

Pros and cons of each technology are discussed. Two main aftertreatment system setups are considered. The effects of catalyst size and catalyst degradation are briefly commented.

3. Emission Control Technologies for Heavy-Duty Vehicles, vol. 3: Development of On Board Diagnostics Systems [5] (2002), Final report

Joint effort by: MIRA Ltd, United Kingdom, PBA, United Kingdom, LAT/AUTH, Greece, TU Graz, Austria, TNO Automotive, Netherlands, Vito, Belgium

OBD system overviewed. Mainly exhaust gas aftertreatment systems and their modifications are described with a focus on possible malfunctions and diagnostics.

- (a) Diesel Particulate filters
- (b) NO_x Adsorbers and Selective Catalytic Reduction
- (c) Exhaust Gas Recirculation systems

4. Detailed Modelling and Simulation of Automotive Exhaust NO_x Reduction Over Rhodium Under Transient Lean-Rich Conditions (2009), Dissertation

Qingyun Su, M.Sc.

 NO_x - PM trade-off is described as well as a historical overview of emission regulations. Also properties of catalytic exhaust NO_x after-treatment systems are presented. Discussed technologies:

- (a) NH_3 -SCR for lean NO_x reduction
- (b) HC-SCR for lean NO_x reduction
- (c) NO_x Storage and Reduction (NSR) Catalyst
- (d) Nakatsuji-type cyclic NO_x decomposition catalyst

Current problems of SRC are discussed.

5. Diesel Engine Emissions and Their Control [10] (2008), Article

Tim Johnoson

Overview of emission regulatory development concerning light and heavy-duty vehicles. Currently used measures to abate armful content in exhaust gas described. Following technologies discussed:

- (a) EGR
- (b) DPF
- (c) SRC and conventional approaches
- (d) LNT and its shortcomings

Proposal for suitably sized urea supply on board, which allows resupply during lubricate-oil changes, is presented. The fact that the European catalysts are vanadium based and Japanese catalysts are zeolite as well as comparison of these setups is revealed. Urea thermal decomposition issues are addressed with usage of bypass heater as possible solution. NH_3 slip catalyst is mentioned. Urea packaging issues are discussed, with proposal of solid urea-storing cartridge. Combined LNT and SCR setup is briefly described. DPF and DOC are also discussed with focus on soot loading and ash build-up.

6. Particulate Matter and NO_x Exhaust Aftertreatment Systems [9] (2007), Article

Jürgen Schnitzler

Overall view of aftertreatment technologies with their pros, cons and comparison is presented:

- (a) DOC
- (b) DPF
- (c) SCR
- (d) LNT

Reveals that the LNT+SRC concept is proposed by some automotive manufacturers. An aftertreatment setup with $DeNO_x$ system placed upstream of CDPF is considered as more beneficial than other setups for light-duty applications. Functional issues of different aftertreatment setups are discussed. Combined particulate and $DeNO_x$ aftertreatment systems are presented. Proposed setups are simulated and obtained results are discussed.

7. Engines and Exhaust After Treatment Systems for Future Automotive Applications [8] (2006), Article

Ulrich G. Alkemade, Bernd Schumann

Contains brief overview of catalytic aftertreatment technology; features of presented systems as well as corresponding markets:

- (a) TWC (mainly for gasoline engines)
- (b) LNT (light-duty GDI/diesel engines)
- (c) SRC with OC (heavy-duty diesel engines)
- (d) DPF (active and passive regeneration process)

Corresponding sensors for each technology are mentioned. Brief description of LNT functionality is showed. Modern SCR catalyst can incorporate the function of hydrolyzing catalyst for urea decomposition.

APENDIX A. BACKGROUND RESEARCH

8. Automobile Exhaust Catalysts [15] (2001), Article

Ronald M. Heck, Robert J. Farrauto

Overview of catalytic technology development over past 30 years is presented. Overview of emission control technologies for abatement of cold start emissions is mentioned. Leading solution: close-coupled catalyst is presented. The Diesel Oxidization Catalysts and the Diesel Particulate Traps are discussed.

9. Low Emission Diesel Particulate After Treatment System Development for Trucks in Japanese City Driving (2004), Article

Takehiko Morozumi, Shigeru Yamamori, Kazunari Komatsu, Yasuaki Unno

Innovative two-stage DPF aftertreatment system for increased low temperature PM filtering proposed. The DOC installed on account of testing a CRT method for additional NO_x abatement. An in-use light truck is used for new DPF system retrofit. Evaluation of results shows substantial improvement of emissions of given vehicle.

A.1.2 Selective Catalytic Reduction (SCR)

1. Urea-SCR in Automotive Applications [12] (2004), Article

Pär L. T. Gabrielsson

Description of SRC (extruded/coated) catalysts and their comparison. Several various catalytic system setups are presented with focus on increased NO_x reduction. Reduction agent selection and catalyst durability are discussed. The reduction activity is explained in various temperature areas for different SCR catalyst. Finally two different models that occur in literature are compared.

NO_x Self-Inhibition in Selective Catalytic Reduction with Urea (ammonia) Over a Cu-zeolite Catalyst in Diesel Exhaust (2002), Article

Lifeng Xu, Robert W. McCabe, Robert H. Hammerle

Chemical point of view. The mechanism of the self-inhibition process, which is likely caused by competitive adsorption of ammonia and NO_x , is described in detail.

3. Lean-burn Catalysts From the Perspective of a Car Manufacturer. Early Work at Volkswagen Research (2004), Article

Axel König, Wolfgang Held, and Thomas Richter

Development of aftertreatment technologies from point of view of a car manufacturer. Focused on HC reactant agent. Several different materials for SRC catalyst fabrication presented. LNT briefly noted.

A.1.3 Diesel Particulate Filter

1. Ceramic Diesel Particulate Filters [14] (2005), Article

Joerg Adler

The Diesel Particulate Filters are presented. Process of the particle filtration and regeneration are described. An ash storage phenomenon is explained. Several different materials suitable for DPF fabrication are compared.

2. Analytical Modelling of Cyclone Separator as a Diesel Soot Particulate Filter with Inner and Outer Vortex Effect (2007), Article

N. Mukhopadhyay, P. K. Bose, R. K. Chakrabarti, A. K. Das

A brand new solution for the DPF is proposed. The main idea consists of usage of a cyclone separator and vortex effect. PM caused health risks briefly described. The proposed cyclone DPF system is analytically modeled and results are discussed.

3. Heat-Integrated Reactor Concepts for Catalytic Reforming and Automotive Exhaust Purification [16] (2007), Article

Grigorios Kolios, Achim Gritsch, Arístides Morillo, Ute Tuttlies, Jens Bernnat, Frank Opferkuch, Gerhart Eigenberger

The coupling of endothermic and exothermic reactions explained. The TWC and LNT catalytic systems briefly noted. Thermal processes in DFP during filter regeneration broadly explained. New integrated exhaust gas purification approach proposed.

4. Performance Assessment of Catalyzed Diesel Particulate Filters (2002), Article

S. Skopa, P. Baltzopoulou, C. Altiparmakis, E. Papaionannou, D. Zarvalis and A. G. Konstandopoulos

Overview of available materials and geometric configurations of the DPFs. Temperature effect on permeability, permeability measurement, loading behavior of filter, filter efficiency and filter regeneration briefly described.

A.1.4 Diesel Oxidation Catalyst

1. Palladium Use in Diesel Oxidation Catalysts [20] (2009), Article

Johnson Matthey

Brief overview of automotive catalyst development. The DOC structure and function briefly described. Focused mainly on usage of palladium in DOC.

2. Diesel Oxidation Catalyst [19] (2004), Article

Author Unknown, Washington State University Extension Energy Program

Function of the Diesel Oxidation Catalyst as well as its cost and other related issues are briefly described.

A.2 Exhaust gas aftertreatment modeling methods and control

Collected materials that are relevant to the studied topic are briefly reviewed for the purpose of gaining an insight into the modelling and control of aftertreatment system issues.

A.2.1 General Topics

1. Is Closed-Loop SCR Control Required to Meet Future Emission Targets? (2007), Article

Frank Willems, Robert Cloudt, Edwin van den Eijnden TNO, Bram de Jager and Wiebe Boomsma from Eindhoven University of Technology and Ignace van den Heubel from DAF Trucks

Writing proposes Closed-Loop as an alternative control method instead of widely used Open-Loop control method. Comparison of features (both pros and cons) of introduced control technologies is presented. Cross sensitivity of current NO_x sensors is reviewed. NH₃ storage is viewed in relation to control. Furthermore, the need of Integrated Emission Management is pointed out. TNO proprietary simulation tool is mentioned.

2. Ammonia Sensor for Closed-Loop SCR Control (2008), Article

Da Yu Wang, Sheng Yao, Mark Shost, Joon-Ho Yoo, David Cabush and David Racine, Delphi Corporation, Robert Cloudt and Frank Willems, TNO Automotive

The importance of NH_3 sensor of corresponding quality for accurate and robust CL control is pointed out. Features of current ammonia sensors are reviewed. NH_3 sensor-based control strategies of SRC catalyst are proposed. Given control strategies are simulated by using TNO's SCR system model and results discussed.

3. 0D Modelling: A Promising Means for After-treatment Issues in Modern Automotive Applications (2009), Article

G. Mauviot, F. Le Berr, S. Raux, F. Perretti, L.M. Malbec and C. N. Millet

Catalysis aftertreatment systems are considered as the most promising for future application. 0D-modelling is proposed as relevant approach to develop reasonably accurate and time-consuming models. Approach based on bond graph theory. The different aftertreatment systems described in relation with current and future Euro regulations. Currently used models are described in brief and 0D modelling is more deeply described. Models of TWC, NO_x trap and DPF are presented.

4. Modelling and Control of Automotive Catalysts (2001), Dissertation

Stephen James Cornelius

Modelling and experiments of automotive catalysts. Work is focused on oxygen storage capacity. Detailed literature review included.

5. Detailed Modelling and Simulation of Automotive Exhaust NO_x Reduction Over Rhodium Under Transient Lean-Rich Conditions (2009), Dissertation

Qingyun Su, M.Sc.

Description of processes on a rhodium based catalytic NO_x decomposition/reduction system operated under periodic lean/rich conditions are considered. Described system kinetics are simulated in DETCHEM. Detailed description of reaction mechanism is presented.

6. Development and Application Range of Mathematical Models for 3-way Catalytic Converters (1996), Article

G. C. Koltsakis, P. A. Konstantinidis, A. M. Samatelos

Innovative 2-D TWC model described in detail. Innovations concerning catalytic transient behavior, the reaction kinetics and solution procedure proposed. Oxygen storage submodel attached. Detailed description of phenomena involved in TWC operation. Rate equation coefficients expressed.

7. Modelling of Catalytic Exhaust Aftertreatment Systems: From Laboratory Reactor Data to Successful Prediction of Emissions From Vehicles (2009), Article

F. Ekström, F. Wallin, A. Fathali, G. Russ

Models of TWC for virtual full-driving tests presented on proprietary software SiKat. Underlying calculus described very briefly. Simulation of oxygen storage and catalyst aging noted.

A.2.2 Selective Catalytic Reduction (SCR)

1. NO_x Modelling of a Complete Diesel Engine/SCR System (2007), Licentiate Thesis

Claes Ericson

The work contains brief introduction to emission regulation and SRC issues. The focus of work is a diesel engine model. Also contains adaptive model of SRC catalyst with underlying analysis and equation calculus. Adaptive model consists of two switched submodels. Switching is controlled by the measured temperature.

2. A State-Space Simplified SCR Catalyst Model for Real Time Applications (2008), Article

Claes Ericson

Two models of SRC catalyst described (very similar as it is in Claes Ericson Licentiate Thesis). One model is more complex, the other is simplified regarding its usage for control. Theoretical and mathematical background included.

3. Monitoring, Feedback and Control of Urea SCR Dosing Systems for NO_x Reduction: Utilizing an Embedded Model and Ammonia Sensing (2008), Article

Mark Shost, John Noetzel, Ming-Cheng Wu, Tanto Sugiarto, Todd Bordewyk, Gary Fulks and Galen B. Fisher

Review. Monitoring and control system for SRC urea dosing and NH_3 sensing after SRC for closed-loop control is introduced. Proposed system is based on 1D SRC model, which is briefly described with underlying calculus. Calibration of obtained model is described subsequently. Test cell setup aftertreatment system mentioned. Advantage of closed-loop control is presented.

4. A Simplified Catalytic Converter Model for Automotive Coldstart Applications with Adaptive Parameter Fitting (2006), Contribution to symposium

Pannag R Sanketi et al., University of California Berkeley, M. Wilcutts, T. Kaga, Toyota Motor Engineering and Manufacturing, North America

Review of model related to coldstart conditions is presented. Simple controloriented model introduced. Model consists of three discrete states and one continuous state. States are related to the engine coldstart phases. Thermal submodel and static efficiency submodel described in detail. Results showed better model accuracy hence the evaporation of water is taken into account.

5. Mathematical modelling of catalytic exhaust systems for EURO-3 and EURO-4 emissions standards (2001), Article

G. Pontikakis and A. Stamatelos

Modelling based on Langmuir-Hinshelwood kinetics with necessary improvements is presented. Best fit model parameter tuning is used for increasing accuracy of the model. Modelling of aged catalysts briefly described.

6. SCR-DeNO_x for Diesel Engine Exhaust Aftertreatment: Unsteady-State Kinetic Study and Monolith Reactor Modelling (2004), Article

Cristian Ciardelli, Isabella Nova, Enrico Tronconi, Brigitte Konrad, Daniel Chatterjee, Karlheinz Eckeb, Michel Weibel

Chemical processes (adsorption-desorption) of NO, NH_3/O_3 regarding SRC-DeNO_x aftertreatment systems are described. Mass balance equations presented.

7. Transient Modelling of a HC-SCR Catalyst for Diesel Exhaust Aftertreatment (2003), Article

Björn Westerberg, Christian Künkel, C.U. Ingemar Odenbrand

The SRC with hydrocarbon reagent is presented instead of classical approach with urea reagent. The full catalyst model is presented, including reaction kinetics (Langmuir-Hinshelwood) and equations for mass and heat transfer. Mechanistic aspects are discussed and related to other studies.

8. Model Based Control of SCR Dosing and OBD Strategies with Feedback from NH₃ Sensors (2009), Article

Andrew Herman, Ming-Cheng Wu, David Cabush and Mark Shost

Work presents the model based control system for SRC urea dosing. Modelling includes SRC chemistry equations. NH_3 sensor is used for closed-loop control strategy. Adaptive control algorithm, which enables compensation of SRC catalyst and/or ammonia sensor aging, is presented.

9. Modelling of an SCR Catalytic Converter for Diesel Exhaust After Treatment: Dynamic Effects at Low Temperature (2005), Article

E. Tronconi et al.

Detailed description of SRC model with innovative approach to low temperature dynamic effects is presented. Experiments with vanadium SRC catalyst discussed. Rate model is derived with a number of underlying rate and chemical equations presented.

A.2.3 Diesel Particulate Filter (DPF)

1. Some Empirical Observations on Diesel Particulate Filter Modelling and Comparison between Simulations and Experiments (2000), Article

P. Versaevel, H. Colas, C. Rigaudeau, R. Noirot, G. C. Koltsakis, A. M. Stamatelos Improved DPF modelling approach presented. Special emphasis is given to the pressure drop model. Particulate layer permeability is discussed. Regeneration process model described in detail with and without presence of fuel additives.

2. Modes of Catalytic Regeneration in Diesel Particulate Filters (1997), Article

Grigorios C. Koltsakis and Anastasios M. Stamatelos

Mathematical 1D model of DPF introduced in detail and influence of fuel additives on regeneration process studied. Regeneration process described in relation to the space velocities. Soot composition briefly described. Mathematical model extension discussed.

3. A 2-D Diesel Particulate Regeneration Model (200?), Article

Author unknown

Brief introduction to DPF function. Overview of DPF model literature. 2D DPF model presented including underlying equation calculus.

A.2.4 Diesel Oxidation Catalyst (DOC)

1. Fundamental Three Dimensional Modelling and Parameter Estimation of a Diesel Oxidation Catalyst for Heavy Duty Trucks, (2009), Article

Anders Holmqvist

Extensive 3D DOC model described in detail. Simulation of model in COMSOL software using finite elements method carried out. Model optimized in MATLAB.

2. Model-based Control Design of a Diesel Oxidation Catalyst (2009), Article

Olivier Lepreux, Yann Creff, Nicolas Petit

1D distributed parameters model of DOC introduced. Underlying equations described in detail. Several control strategies applied including PI, PI(D); both with feedforward terms and finally Smith Predictor. Comparison of results included.

3. Modelling and Simulation of a Diesel Oxidation Catalyst Used in a NO_x Storage and Reduction System for Heavy Duty Trucks (2008), Article

Enric Senar Serra

Two DOC models with underlying equation calculus introduced (Equilibrium limiting model and Kinetic limiting model). Both models showed different temperature properties, but none covered whole exhaust gas temperature range.

4. Warm-up Strategy for a Diesel Oxidation Catalyst, (2009), Article

Olivier Lepreux, Yann Creff and Nicolas Petit

Warm-up strategy, which is based on HC pulse injection as a control signal, for DOC is proposed. Research based on simple 1D thermal DOC model with distributed parameters. Warm-up strategy parameters studied in detail. Results presented.

5. Intra-channel Mass and Heat-Transfer Modelling in Diesel Oxidation Catalysts (2001), Article

Kalyana Chakravarthy, C. S. Daw, J. C. Conklin

Speculates that intra channel gas flow in DOC is not laminar due to roughness and washcoat porosity. That causes non-negligible deviation of model response from real measurements. Dependence between Reynolds, Nusselt and Sherwood numbers is discussed.

Apendix B

Content of the Attached CD

The attached CD contains an electronic version of this thesis, as well as published and unpublished figures. The source codes and models are treated as confidental and are property of the Honeywell company.

- Directory 1: Figures
- Directory 2: Thesis