ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL

MODEL-BASED SIMULATION AND OPTIMIZATION OF AN SCR SYSTEM FOR A HEAVY-DUTY DIESEL ENGINE

M.Sc. THESIS

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ISTANBUL TEKNİK ÜNİVERSİTESİ ★ LİSANSÜSTÜ EĞİTİM ENSTİTÜSÜ

AĞIR VASITA DİZEL MOTORU İÇİN SCR SİSTEMİNİN MODEL TABANLI SİMÜLASYON VE OPTİMİZASYONU

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Muhammed Enes Karagöz, a M.Sc. student of İTU Graduate School student ID 503221711, successfully defended the thesis/dissertation entitled "MODEL-BASED SIMULATION AND OPTIMIZATION OF AN SCR SYSTEM FOR A HEAVY-DUTY DIESEL ENGINE", which he prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below

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To my family,

FOREWORD

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June 2025 Muhammed Enes Karagöz
(Mechanical Engineer)

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ABBREVIATIONS

AI	: Artificial Intelligence
ASC	**:** Ammonia Slip Catalyst
DOC	: Diesel Oxidation Catalyst
DPF	: Diesel Particulate Filter
ECU	: Engine Control Unit
EGR	: Exhaust Gas Recirculation
EPA	: Enviromental Protection Agency
FBC	: Feedback Control
FFC	: Feedforward Control
HIL	: Hardware in the Loop
MBD	: Model Based Development
MPC	: Model Predictive Control
NH_3	: Ammonia
NO_x	: Nitrogen Oxides
OBD	: On Board Diagnosis
RDE	: Real Driving Emissions
SCR	: Selective Catalytic Reduction
TP	:Tail Pipe
WHO	: World Health Organization
WHSC	: World Harmonized Stationary Cycle
WHTC	: World Harmonized Transient Cycle

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MODEL-BASED SIMULATION AND OPTIMIZATION OF AN SCR SYSTEM FOR A HEAVY-DUTY DIESEL ENGINE

SUMMARY

This study aims to develop and optimize a simulation model of a Selective Catalytic Reduction (SCR) system for a 12.7-liter heavy-duty diesel engine that complies with Euro VI emission standards under transient operating conditions. Euro VI regulations have significantly tightened nitrogen oxide (NO_x) emission limits for heavy-duty engines. Achieving such high NO_x conversion efficiency under real driving conditions poses a considerable engineering challenge. Therefore, it is critically important to carefully design advanced aftertreatment solutions like SCR. In this context, modeling the performance of the SCR system under dynamic operating conditions, such as the World Harmonized Transient Cycle (WHTC), provides valuable insights into system behavior and optimization possibilities.

In this study, the SCR system was modeled in MATLAB/Simulink, including both its physical components and control algorithms. The developed comprehensive simulation model covers the NO_x emission source at the engine outlet, the AdBlue injection system, and the behavior of the SCR catalyst. Data obtained from WHTC test cycles were used for model calibration and validation. This ensured that the model could accurately reflect the emission behavior of the engine and the catalyst conversion performance under transient conditions.

Model validation was carried out by comparing simulation results with experimental data. During this process, key performance indicators such as NO_x concentration at the exhaust outlet and AdBlue consumption were evaluated. The simulation results largely aligned with the experimental data obtained at different engine load and speed conditions throughout the transient cycle. The model successfully predicted NO_x reduction efficiency and urea consumption with near-realistic accuracy. This confirms that the model effectively captures the dynamic behavior of the SCR system and its control under real-world driving conditions.

Following validation, a series of parametric studies was conducted to examine how different design and operating parameters affect SCR performance. Parameters such as catalyst volume, injector (AdBlue) capacity, catalyst aging, and dosing control strategy were systematically varied. The effects of each variable on NO_x conversion efficiency and AdBlue consumption were analyzed. The analyses investigated the impacts of catalyst size, injector capacity, and catalyst aging on NO_x emissions and the required AdBlue dosing amounts.

The results highlight the benefits of the Model-Based Development (MBD) approach in designing and developing SCR systems. By using the simulation model, design optimizations and control improvements can be rapidly evaluated without the need for

comprehensive physical prototypes. This allows a wide range of scenarios to be analyzed cost-effectively in a virtual environment. Through this approach, engineers can determine optimal system configurations and control strategies that ensure maximum NO_x reduction while minimizing excessive AdBlue consumption and preventing ammonia slip. Thus, strict emission regulations can be met with significant time and resource savings.

In conclusion, this thesis presents a comprehensive SCR system model and demonstrates its capability to effectively guide the design and optimization of exhaust systems for heavy-duty engines. The developed model serves as a powerful tool for predicting system behavior under transient operating conditions and guiding design decisions in an informed manner. Overall, this study contributes to the development of effective SCR system solutions for Euro VI compliance and emphasizes the role of simulation and model-based methods in modern automotive engineering.

AĞIR VASITA DİZEL MOTORU İÇİN SCR SİSTEMİNİN MODEL TABANLI SİMÜLASYON VE OPTİMİZASYONU

ÖZET

Bu çalışma, Euro VI emisyon standartlarını karşılayan 12,7 litrelik bir ağır vasıta dizel motoru için Selective Catalytic Reduction (SCR) sisteminin model tabanlı simülasyonu ve optimizasyonunu kapsamaktadır. Özellikle değişken ve dinamik motor çalışma koşullarında SCR sisteminin davranışlarının doğru şekilde modellenmesi ve geliştirilmesi hedeflenmiştir. Euro VI düzenlemeleri, dizel motorlu ağır vasıtalar için azot oksit (NO_x) emisyon limitlerini önemli ölçüde düşürerek sektörde çevreye duyarlı teknolojilere olan ihtiyacı artırmıştır. Bu sınırları sağlamak yalnızca motor içi stratejilerle değil, aynı zamanda egzoz sonrası arıtma sistemlerinin etkinliğiyle de yakından ilişkilidir. Bu bağlamda, SCR sistemleri, NO_x emisyonlarının azaltılmasında en yaygın kullanılan ve en etkili teknolojilerden biri olarak öne çıkmaktadır. Ancak gerçek sürüş koşullarında, SCR sistemlerinin yeterli düzeyde NO_x dönüşüm verimliliği sağlaması oldukça karmaşık bir mühendislik problemi olarak karşımıza çıkmaktadır.

Günümüzde SCR sistemlerinin modellenmesi ve kontrolü üzerine yapılan çalışmalar, üç temel eksen etrafında şekillenmektedir: modelleme - doğrulama, kontrol stratejileri ve sistem optimizasyonu. Literatürde motor modelleri ile entegre edilen SCR sistemleri, dinamometre verileriyle karşılaştırıldığında %5'in altında hata oranları ile yüksek doğrulukta sonuçlar vermiştir. Kontrol stratejileri alanında ise, ilk dönemde geliştirilen açık çevrim veya geri besleme temelli kontrol yapılarının yerini, günümüzde ileri besleme - geri besleme kombinasyonları almış; çok amaçlı optimizasyon teknikleriyle hem NO_x dönüşüm verimliliği hem de amonyak slip'i dengelenmiştir. Sistem seviyesinde optimizasyon çalışmaları, donanım içeren test sistemleri (HIL) ve sanal kalibrasyon ortamları ile desteklenmiş, bu sayede prototip üretim süreci önemli ölçüde hızlandırılmıştır. Mevcut çalışma, literatürde önerilen bu üç eksenin bir araya getirildiği bütünleşik bir modelleme ve analiz örneği sunmaktadır.

Bu zorluğu aşmak amacıyla geliştirilen model, World Harmonized Transient Cycle (WHTC) gibi gerçek sürüşe yakın test koşullarında sistem davranışlarını anlamayı ve değerlendirmeyi hedeflemiştir. WHTC çevrimi; düşük, orta ve yüksek motor yükleri ile devir aralıklarını içeren geniş kapsamlı bir test prosedürüdür ve bu sayede SCR sisteminin her koşuldaki tepkileri detaylı şekilde analiz edilebilmektedir. Geliştirilen modelin amacı yalnızca sistem tepkilerini tahmin etmek değil, aynı zamanda kontrol stratejilerinin etkinliğini test etmek ve sistem parametrelerinin optimizasyonuna katkıda bulunmaktır.

Modelleme çalışması MATLAB/Simulink platformunda gerçekleştirilmiş ve SCR sistemine ait fiziksel bileşenlerin yanı sıra kontrol algoritmaları da entegre edilmiştir. Sistem, motor çıkışında oluşan NO_x miktarını temel alarak dozajlama miktarını belirleyen bir kontrol yapısına sahiptir. Simülasyon modeli; AdBlue enjeksiyon sistemi, termal parçalanma ve hidroliz reaksiyonları, amonyak oluşumu ve SCR katalizöründeki kimyasal dönüşüm süreçlerini dikkate alarak oluşturulmuştur. NH_3'ün gaz fazında oluşumu, katalizör yüzeyine taşınımı, adsorpsiyonu, yüzey reaksiyonları ve desorpsiyonu gibi adımlar modelde ayrı ayrı ele alınmıştır. Ayrıca sıcaklık, basınç, egzoz debisi gibi dış parametrelerin reaksiyon verimliliğine etkisi de modele entegre edilerek, fiziksel gerçeklik artırılmıştır.

Modelin kalibrasyon ve doğrulama süreci, dinamometre testlerinden elde edilen deneysel veriler kullanılarak gerçekleştirilmiştir. WHTC çevrimi boyunca toplanan veriler ile simülasyon çıktıları karşılaştırılmış; egzoz çıkışındaki NO_x konsantrasyonu, AdBlue tüketimi ve tailpipe NO_x değerleri analiz edilmiştir. Elde edilen sonuçlar, simülasyon çıktılarının deneysel verilerle büyük ölçüde örtüştüğünü göstermiştir. Tüm bu parametreler için %5'in altında hata oranları gözlenmiş ve bu doğrulama sonuçları, geliştirilen modelin dinamik koşullarda yüksek tahmin gücüne sahip olduğunu ortaya koymuştur.

Doğrulama sürecinin ardından, SCR sisteminin performansını etkileyen çeşitli parametreler üzerinde sistematik bir parametrik analiz gerçekleştirilmiştir. Bu analizlerde katalizör hacmi, enjektör kapasitesi, katalizör yaşlanması ve dozaj kontrol stratejileri gibi faktörler ele alınmış ve bu parametrelerin NO_x dönüşüm verimliliği ile AdBlue tüketimi üzerindeki etkileri detaylı olarak incelenmiştir. Örneğin, katalizör hacmi arttıkça tepkime için daha uzun bir temas süresi elde edilmekte ve dönüşüm verimliliği artmaktadır. Ancak bu durum aynı zamanda sistem hacmini ve maliyeti de artırmaktadır. Benzer şekilde, enjektör kapasitesinin yüksek olması hızlı tepkime avantajı sağlarken, fazla AdBlue kullanımı sonucunda amonyak kaçağı (NH_3 slip) riskini artırmaktadır. Yaşlanmış katalizör simülasyonları ise reaksiyon hız sabitlerinin düşmesiyle NO_x dönüşüm verimliliğinin azaldığını göstermektedir. Bu analizler, tasarım kararlarının sistem performansı üzerindeki etkilerini daha iyi kavramayı sağlamıştır.

Bu çalışmada SCR sistemi içerisinde gerçekleşen kimyasal reaksiyonlar ve bu süreçlerin katalizör üzerindeki kinetiği de detaylı bir biçimde ele alınmıştır. SCR sistem performansı, NH_3'ün NO ve NO_2 ile uygun sıcaklık aralığında ve yeterli yüzey temas süresi içinde etkin biçimde reaksiyona girmesine bağlıdır. Reaksiyonlara yönelik termodinamik ve kinetik yaklaşımlar kullanılarak sistemin davranışı doğru şekilde modellenmiş; adsorpsiyon, yüzey reaksiyonu ve desorpsiyon adımları dahil edilmiştir. Bu yaklaşım, yalnızca sistem çıktılarının değil, aynı zamanda mikroskobik süreçlerin de fiziksel gerçekliğe uygun biçimde temsil edilmesini sağlamıştır.

Geliştirilen model yalnızca mevcut sistemlerin analizini gerçekleştirmekle kalmayıp, aynı zamanda gelecekteki araştırma ve geliştirme çalışmalarına da temel oluşturmaktadır. Bu doğrultuda, modelin gelecek çalışmalarda üç ana eksende geliştirilmesi planlanmaktadır: Gerçek zamanlı HIL (Hardware-in-the-Loop) uygulamalarına entegre edilerek kontrol algoritmalarının test edilmesi, katalizör yaşlanmasının zamanla reaksiyon kinetiğine etkisinin modellenmesi, termal yönetim stratejileri ile sistemin düşük sıcaklıklardaki performansının iyileştirilmesi. Bu gelişmelerle birlikte, modelin hem akademik hem de endüstriyel uygulamalarda kullanımı yaygınlaşacaktır.

Simülasyon temelli analizler, model tabanlı geliştirme (Model-Based Development - MBD) yaklaşımının mühendislik süreçlerine sağladığı katkıyı açıkça ortaya koymaktadır. Fiziksel prototiplere ihtiyaç duymadan farklı senaryoların ve tasarım kombinasyonlarının düşük maliyetle değerlendirilmesine olanak tanıyan bu yöntem, geliştirme sürecini hızlandırmakta ve kaynak kullanımını optimize etmektedir. Geliştirilen model, yalnızca akademik bir değerlendirme aracı değil, aynı zamanda endüstride kullanılabilecek pratik bir simülasyon platformu olarak da işlev görebilecek niteliktedir.

Sonuç olarak, bu tez kapsamında geliştirilen kapsamlı SCR simülasyon modeli, Euro VI emisyon düzenlemelerine uyumlu ağır vasıta motorlarında egzoz sonrası arıtım sistemlerinin etkinliğini değerlendirmek, kontrol stratejilerini test etmek ve tasarım optimizasyonlarını gerçekleştirmek için güçlü bir mühendislik aracı sunmaktadır. Gerçekleştirilen doğrulama çalışmaları, modelin dinamik koşullarda bile güvenilir tahminler sağlayabildiğini kanıtlamış; parametrik analizler ise sistem performansını etkileyen unsurlar hakkında detaylı öngörüler sunmuştur. Bu yönüyle çalışma, modern otomotiv mühendisliğinde model tabanlı yaklaşımların önemine ve emisyon kontrol teknolojilerinin geliştirilmesinde oynadığı role dikkat çekmektedir.

1. INTRODUCTION

Air pollution remains one of the most serious environmental problems threatening public health. According to the World Health Organization (WHO), approximately seven million people worldwide die each year due to causes related to air pollution, and more than 90% of the global population breathes air that exceeds established limit values [1]. Among these pollutants, nitrogen oxides (NO_x) hold particular importance due to their harmful effects on both human health and the environment. NO_x contributes to respiratory diseases, acid rain, and the formation of photochemical smog; especially in industrialized regions, road transportation and internal combustion engines account for a significant share of anthropogenic NO_x emissions.

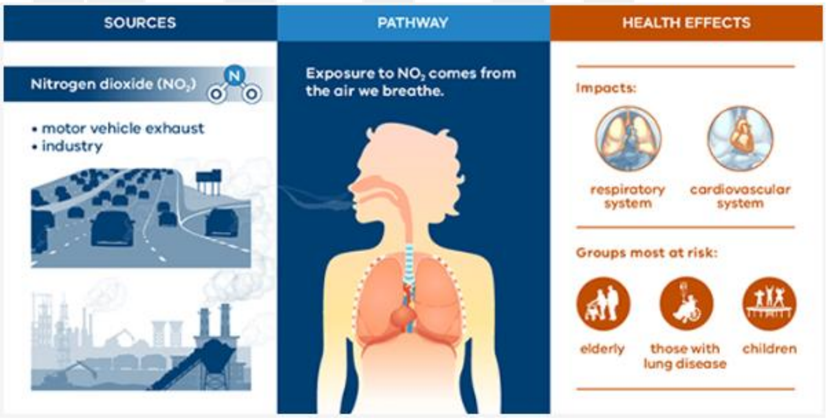

Figure 1.1 : NOx emissions health effects. Retrieved from [2].

To reduce the effects illustrated in Figure 1.1, legislation has progressively moved toward stricter emission standards over time. In Europe, the Euro VI regulation currently in force for heavy-duty engines limits NO_x emissions to 0.4 g/kWh under steady-state conditions (WHSC) and 0.46 g/kWh under transient cycle conditions (WHTC). Additionally, supplementary limits have been introduced for ammonia (NH_3) slip [3]. Meeting such stringent thresholds under real-world driving conditions is made possible through the use of Selective Catalytic Reduction (SCR) technology (Figure 1.2). SCR systems reduce NO_x in the exhaust gas by converting them into N_2 and H_2O, using NH_3 derived from a urea solution (AdBlue) over V_2O_5 or Cu/Fe-zeolite catalysts.

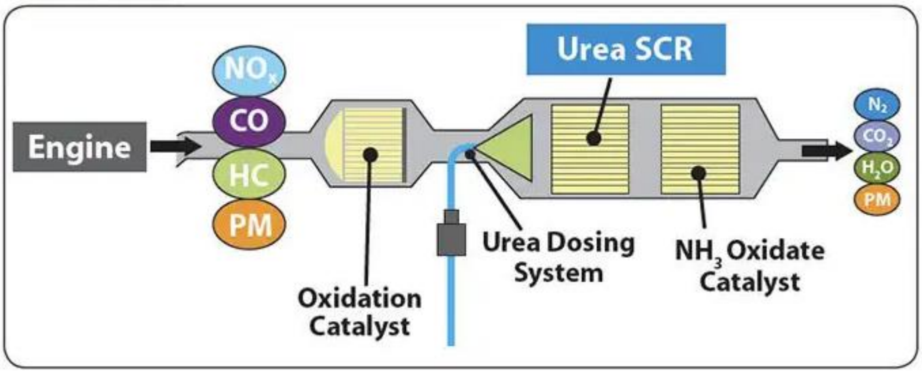

Figure 1.2 : SCR System. Retrieved from [4].

Although SCR systems are a mature technology in commercial applications, both their hardware components and control algorithms still require extensive and costly experimental efforts for each new engine platform, catalyst formulation, or calibration update. In this context, Model-Based Development (MBD) emerges as a cost-effective alternative for the design of engine and emission systems. Through the MBD approach, high accuracy yet computationally feasible simulations allow for the preliminary evaluation of variables such as hardware sizing, ageing scenarios, and injection strategies without the immediate need for dynamometer or vehicle testing.

In the literature, the modeling and optimization of SCR systems have progressed along three main axes. The first is modeling and validation. Using experimental efficiency maps integrated with mean-value engine models, error rates below 5% have been achieved in comparisons with dynamometer data [5].

The second is closed-loop control and calibration. Starting from early model-based feedforward/feedback control architectures, today's systems have evolved into multi-objective optimization frameworks that enable balanced control of both NO_x conversion efficiency and ammonia slip [6].

The third is system-level optimization and virtual calibration. Real-time hardware-in-the-loop (HIL) testing systems [7] and integrated diesel engine/SCR models accelerate the calibration process of SCR systems and improve the effectiveness of virtual calibration methods [8].

An SCR model that has been thoroughly validated using WHTC test data is expected to contribute to the literature, and an integrated framework has been established to simultaneously examine critical parameters such as catalyst volume, injector capacity, and catalyst efficiency (ageing). A clear understanding of these parametric interactions is crucial for predicting end-of-life system performance and determining the optimal SCR hardware package sizing, especially for high-displacement diesel engines.

1.1 Purpose of Thesis

The primary objective of this thesis is to develop an SCR model for a 12.7-liter heavy-duty diesel engine compliant with Euro VI standards, validate its accuracy using experimental data, and analyze system behavior under various hardware and software parameter changes. For this purpose, a physics-based SCR model was developed in the MATLAB/Simulink environment. The model was validated against dynamometer test data in terms of key performance indicators such as NO_x conversion efficiency, tailpipe NO_x (TP NO_x), and AdBlue consumption, with a target error margin of less than 5% for each parameter. After validation, the effects of variables such as SCR catalyst volume, urea injector capacity, and catalyst efficiency on system performance under WHTC cycles were systematically investigated.

The findings obtained within the scope of this thesis aim to demonstrate how the model-based development (MBD) approach can be used to ensure compliance with emission standards while reducing design time. Additionally, the study seeks to contribute to making heavy-duty engines compliant with environmental regulations by providing design guidance for appropriate hardware selection and calibration strategies.

1.2 Literature Review

This section presents a comprehensive review of recent studies and technical publications related to the modeling, simulation, and optimization of Selective Catalytic Reduction (SCR) systems in heavy-duty diesel engines. The aim is to summarize the current state of knowledge and to identify key modeling strategies and control approaches.

1.2.1 Air pollution and the significance of NO_x emissions

Nitrogen oxide (NO_x) emissions from fossil fuel-powered engines have significant negative effects on both the environment and human health. In the atmosphere, NO_x gases contribute to the formation of ground-level ozone and fine particulate matter, triggering photochemical smog problems. Additionally, NO_x mixes with rainwater, causing acid rain that harms ecosystems. From a health perspective, inhalation of NO_x can lead to respiratory tract irritation, worsen asthma attacks, and, in the long term, cause cardiopulmonary diseases [9]. Diesel-powered vehicles, in particular, are among the primary sources of NO_x emissions (Figure 1.3); heavy-duty diesel vehicles contribute substantially to atmospheric NO_x levels [10]. Therefore, controlling NO_x emissions is of great importance, both to improve local air quality and to mitigate global environmental problems.

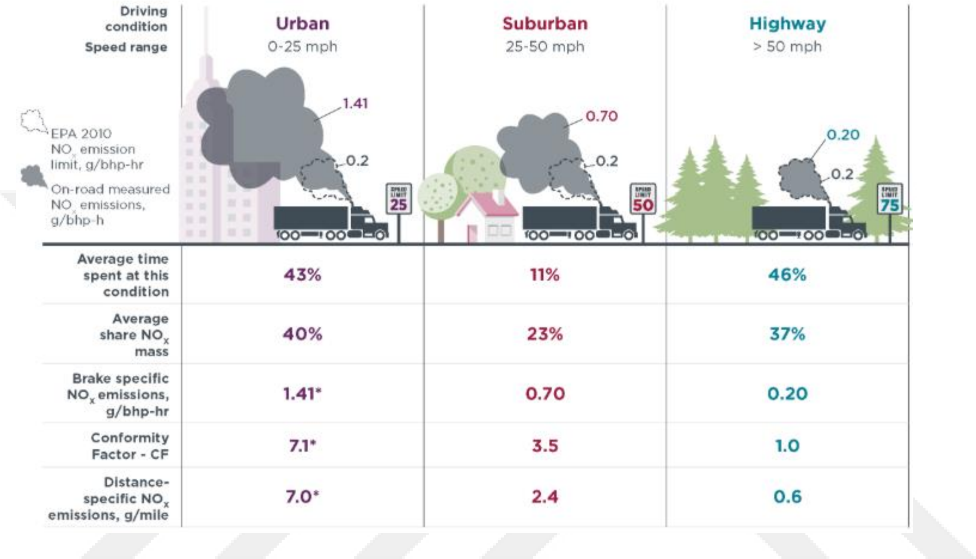

Figure 1.3 : Brake and distance specific NO_x emissions. Retrieved from [11].

1.2.2 Emission regulations and compliance challenges

In order to reduce air pollution, legal regulations limiting vehicle emissions have become increasingly stringent worldwide. In Europe, the Euro standards applied to both light- and heavy-duty vehicles have significantly lowered the NO_x emission limits over the years. For instance, when transitioning from Euro V to Euro VI for heavy-duty diesel engines, NO_x emission limits were reduced by approximately 77%, as seen in Figure 1.4, lowering the upper limit for NO_x in the transient test cycle (WHTC) from around 2.0 g/kWh to 0.46 g/kWh [12]. This dramatic tightening has compelled engine manufacturers to adopt advanced emission control technologies, especially Selective Catalytic Reduction (SCR) systems. As a result, SCR catalysts are now widely used in nearly all heavy-duty diesel vehicles produced after the Euro VI standard to achieve high-efficiency NO_x reduction.

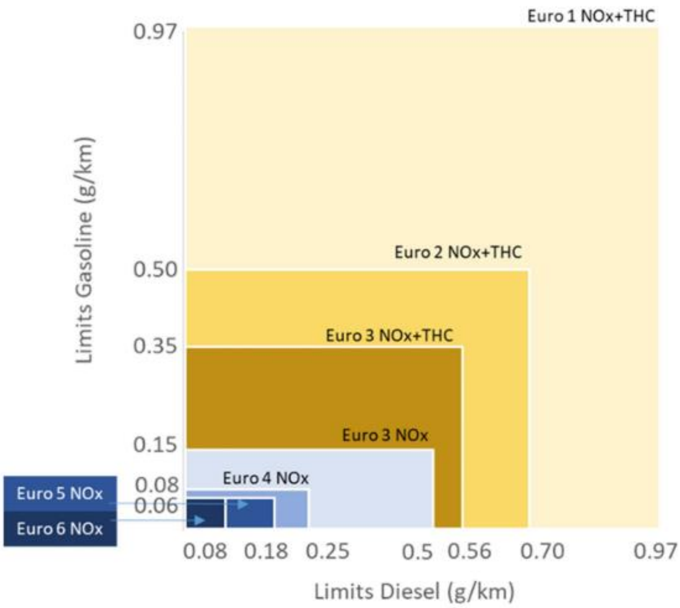

Figure 1.4 : Emission regulation limits. Retrieved from [13].

Ensuring compliance with these regulatory limits under real-world driving conditions, outside of controlled laboratory tests, poses a significant engineering challenge. Maintaining effective NO_x control during off-cycle operation is difficult, and studies have shown that modern diesel vehicles can emit much higher NO_x levels on the road than expected [12]. This is especially true under the Euro VI regulation, where heavy-duty vehicles must pass the World Harmonized Transient Cycle (WHTC) as well as the subsequent Real Driving Emissions (RDE) tests. These test cycles include demanding conditions such as low engine load and low exhaust temperatures, making it harder to consistently keep NO_x emissions below the required limits [10]. As a result, manufacturers have been compelled to develop more advanced SCR systems and to fine-tune engine calibration strategies (e.g., fuel injection adjustments in cold conditions, use of EGR) in an integrated way to comply with Euro VI requirements. In summary, the tightening of emission regulations has driven the need for innovative NO_x reduction technologies and precise control systems.

1.2.3 Basic operating principle and chemistry of the SCR system

Selective Catalytic Reduction (SCR) is an aftertreatment technology designed to convert NO_x emissions from diesel engines into harmless components. In this system, a reducing agent known as urea solution (AdBlue) is injected into the exhaust stream. At high exhaust temperatures, urea undergoes thermal decomposition and hydrolysis reactions to form ammonia (NH_3). The resulting ammonia selectively reacts with NO and NO_2 on the SCR catalyst surface to reduce NO_x gases into nitrogen (N_2) and water (H_2O) [14]. This process occurs despite the oxygen-rich exhaust environment, as NH_3 reacts preferentially with NO_x rather than with oxygen, hence the term "selective". The general chemical equations representing the SCR reactions are as follows:

$$NH_3 + Surface\ Site \leftrightarrow NH_{3\_}S \tag{3.1}$$

$$NH_{3\_}S + O_2 \rightarrow N_2 + H_2O \tag{3.2}$$

$$NO + O_2 \leftrightarrow NO_2 \tag{3.3}$$

$$NH_{3\_}S + NO + O_2 \rightarrow N_2 + H_2O \tag{3.4}$$

$$NH_{3\_}S + NO + NO_2 \rightarrow N_2 + H_2O \tag{3.5}$$

$$NH_{3\_}S + NO_2 \rightarrow N_2 + H_2O \tag{3.6}$$

In addition to the desired reduction reactions between ammonia and NO_x, some unwanted side reactions may also occur. For example, at high temperatures, ammonia can oxidize with oxygen to form NO, or under incomplete reaction conditions, N_2O (nitrous oxide) may be produced. Therefore, for the SCR system to operate efficiently, maintaining the proper NH_3/NO_x ratio within the correct temperature range is critically important.

SCR catalysts are typically produced by coating active catalytic components onto porous ceramic monoliths. The two most common material technologies used in SCR catalysts are vanadium-based (V_2O_5-WO_3/TiO_2) and zeolite-based catalysts (typically zeolites exchanged with Cu or Fe). Vanadium/titania catalysts offer high NO_x reduction efficiency at relatively low temperatures (usually in the 200-400 °C range) and exhibit good resistance to sulfur poisoning. Additionally, thermally stabilized vanadium catalysts, which can withstand short-term exposure to high exhaust temperatures (500-650 °C), are widely used in heavy-duty applications [14]. Zeolite-based catalysts, on the other hand, are increasingly preferred in newer vehicle generations due to their high activity at elevated temperatures (typically above 400 °C) and superior thermal durability. Both catalyst types can achieve NO_x conversion efficiencies exceeding 90% under appropriate conditions [15]. In SCR reactions, the catalyst volume and geometry are also important; increasing the surface area exposed to the exhaust gas and the residence time enhances the NO_x conversion efficiency [16]. Figure 1.5 illustrates the chemical processes that occur during SCR reactions on the catalyst surface.

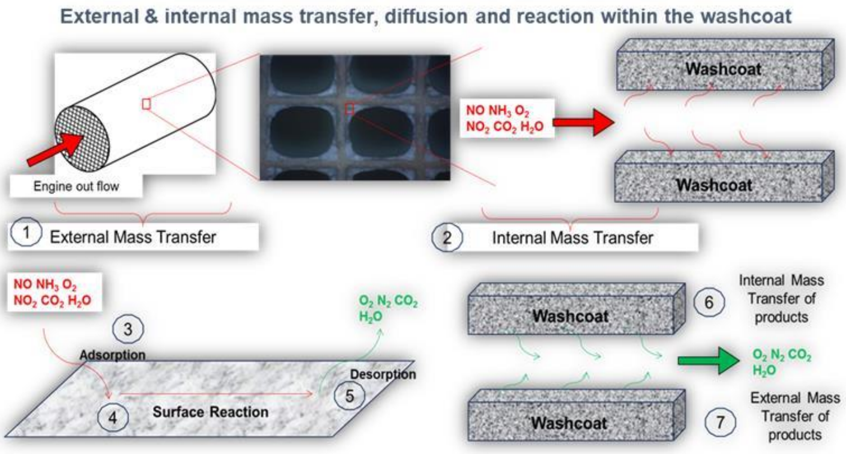

Figure 1.5 : Chemical processes that occur during SCR reactions on catalyst surface.

1.2.4 SCR components

An SCR system operates through the integration of several subcomponents. The main components are as follows: (i) Reductant tank, this tank stores the AdBlue solution, which consists of 32.5% urea and 67.5% deionized water. (ii) Dosing system , controlled by the electronic control unit (ECU), this system includes a pump and injector that spray the urea solution into the exhaust stream. (iii) Catalyst converter, a reactor unit with a ceramic or metallic monolith structure coated with active SCR catalyst material. It is mounted in the exhaust line and provides the environment where the reactions between NH_3 and NO_x take place. (iv) Sensors and control components, NO_x sensors placed before and after the SCR catalyst measure the NO_x concentration to enable feedback control. Other components include temperature sensors that monitor the exhaust gas temperature, and level sensors that track the AdBlue volume.

The SCR system operates in a closed-loop configuration with the ECU, adjusting the dosing amount in real time to ensure high NO_x conversion efficiency while avoiding excessive ammonia injection [17].

The operation sequence of an SCR system proceeds as follows: First, the engine exhaust gas enters a mixing section, if included, where the injected urea solution evaporates due to the hot exhaust flow and is converted into ammonia (NH_3), which is then evenly distributed within the gas stream. This mixture then flows into the SCR catalyst. Here, the NH_3 derived from the urea solution is first adsorbed onto the catalyst surface. On the active surface of the catalyst, the NH_3 reacts chemically with NO and NO_2 present in the exhaust, converting them into harmless nitrogen (N_2) and water (H_2O). Ideally, no NO_x remains in the exhaust gases exiting the catalyst. However, due to control strategies or dynamic operating conditions, a small amount of unreacted NH_3 slip may occur. To prevent this, many heavy-duty SCR systems include an Ammonia Slip Catalyst (ASC) downstream of the SCR catalyst, which oxidizes the remaining NH_3 into nitrogen and water. Additionally, some systems incorporate a Diesel Oxidation Catalyst (DOC) upstream of the SCR to adjust the NO/NO_2 ratio in the exhaust. Increasing NO_2 formation can enhance the SCR reaction efficiency. In summary, an SCR system is designed as an integrated setup that includes reductant injection from the tank, catalytic reactions, and sensor-based feedback control. When properly designed and calibrated, an SCR system can achieve high NO_x conversion efficiency and plays a crucial role in meeting stringent emission regulations such as Euro VI.

1.2.5 Model based development

Today, the Model-Based Development (MBD) approach is widely used in automotive engineering for designing complex powertrain and emission control systems [18]. MBD is based on creating a mathematical model of the real system and simulating it in a computer environment. In this approach, models based on physical principles are developed for systems such as an engine and SCR, and both design and control strategies are tested and optimized on a virtual prototype. This reduces the need for costly and time-consuming physical prototype testing.

The main steps of the model-based design process are as follows: First, a model set is created using equations, formulas, or data-driven methods to represent the system. Then, these models are validated with experimental data to ensure they accurately reflect real system behavior. Using validated models, simulations are carried out, allowing different design alternatives, control algorithms, or operating scenarios to be tested in a virtual environment without needing to run them on real hardware. For example, the performance of an SCR dosing control algorithm under various driving conditions can be evaluated on the model to select the best parameters. With the MBD approach, development cycles are shortened, and costs are reduced.

In areas like automotive exhaust emissions, where conditions are highly variable and complex, the MBD approach offers significant advantages. Tests that are difficult or expensive to conduct on real vehicles can be performed on the model using advanced tools such as Hardware-in-the-Loop (HIL). For instance, in a study by Riccio et al. (2022), zero-dimensional (0D) real-time models were developed for a diesel engine and SCR system. These models were connected to a real engine control unit and operated within a virtual test bench. The results showed that the virtual model produced outputs consistent with experimental data under both steady-state and transient cycles [8]. Such a virtual calibration platform allows advanced control algorithms to be tested on hardware, reducing the need for prototypes and significantly accelerating the development process.

Another reason for the widespread adoption of the MBD approach in the automotive industry is its ability to balance conflicting targets in complex systems. For example, optimizing multiple parameters to reduce NO_x emissions while maintaining fuel economy becomes more manageable with model-assisted search methods. In conclusion, model-based development has become an indispensable tool in modern engineering, both for product development and for meeting regulatory requirements.

1.2.6 SCR modeling studies in the literature

In the literature, numerous studies have focused on the modeling and control of SCR systems. Early research mainly concentrated on simplified models for control purposes and empirical parameter tuning. For example, Song and Zhu (2002) developed a pioneering study on the closed-loop control of a urea-injection-based SCR system, presenting a simple yet effective model capable of capturing SCR dynamics for real-time control [19]. This study demonstrated that using a feedback control strategy, where ammonia dosing is adjusted based on NO_x sensor measurements in the diesel engine exhaust, is feasible. Later, Covassin et al. (2009) proposed a mean-value model of an SCR system integrated into an automotive diesel engine. Their model mathematically represented the complete exhaust system, including engine output, DOC, DPF, and SCR, and was used to simulate control strategies balancing fuel consumption and emission reduction [20]. The study highlighted the benefits of model-based approaches for optimizing the engine and aftertreatment system as a whole.

In the 2010s, the introduction of OBD (On-Board Diagnostics) requirements and more stringent emission regulations spurred the development of SCR models aimed at real-time performance monitoring and fault detection. Su et al. (2011) presented a MATLAB/Simulink-based model that estimated the NO_x conversion efficiency of an SCR system [21]. Their model utilized NO_x sensor data from both the inlet and outlet of the SCR system to calculate instantaneous conversion efficiency. The results demonstrated how a model-based monitoring algorithm could track NO_x reduction performance and detect incorrect dosing or loss of catalyst efficiency in the field, in compliance with Euro V/VI OBD regulations.

Several studies in the literature have focused on optimizing SCR dosing and understanding ammonia storage behavior. For instance, Opitz et al. (2015) used a chemical kinetics-based model to simulate NO_x conversion in SCR catalysts under individually tuned NH_3 dosing strategies. Their study investigated scenarios where separate NH_3 injections were applied to different cylinders or exhaust branches, demonstrating that optimizing dosing distribution can increase NO_x conversion while reducing ammonia slip [22]. Yan et al. (2019) developed a physico-chemical SCR model and performed a multi-parameter optimization that simultaneously adjusted urea dosing and ammonia coverage ratio on the catalyst surface [6]. Their approach showed that even under varying engine operating conditions, it was possible to maximize NO_x conversion while minimizing NH_3 slip. In recent years, many studies have shifted their SCR control targets to directly regulate the ammonia coverage ratio on the catalyst surface [7]. This strategy accounts for the catalyst's dynamic NH_3 storage capacity and enables more precise balancing between NO_x reduction and NH_3 slip.

Real-time implementation-oriented models also hold a significant place in the literature. For example, Riccio et al. (2022) developed detailed engine and SCR models for an off-road diesel engine and operated them under real-time conditions in a hardware-in-the-loop (HIL) setup to perform virtual calibration. This work created a digital twin of the physical engine and aftertreatment system, allowing emission control strategies to be tested under different load profiles in a desktop simulation environment [8]. The results showed strong agreement between simulation outputs and physical measurements, emphasizing that model-based calibration significantly speeds up development. Similarly, Dekate et al. (2021) presented a validated SCR performance prediction model using experimental data, focusing on model-based design and verification processes [5]. Such studies confirm that model-based control approaches can be successfully applied in SCR systems, offering valuable tools for both development and calibration purposes.

In recent years, artificial intelligence and data-driven approaches have also started to appear in the SCR modeling literature. Ronkema (2020) developed a model that used advanced regression techniques to predict NO_x emissions from a diesel engine based on engine sensor data [23]. This study demonstrated that machine learning approaches, alongside traditional physics-based models, can achieve a certain level of accuracy in emissions prediction. On the other hand, Wang et al. (2024) proposed an intelligent optimization algorithm based on multi-model state estimation for SCR systems in diesel engines. This method adjusts the urea injection rate in real time under actual operating conditions, managing to keep NH_3 slip under control while maximizing NO_x conversion efficiency [24]. These results show that, in addition to conventional control strategies, AI-supported optimization methods can also contribute to improving SCR system performance.

In summary, SCR modeling studies in the literature have evolved across a broad spectrum, from basic control-focused models to kinetic simulations, optimization methods, and artificial intelligence applications. Each of these studies offers unique perspectives for the design and control of SCR systems and contributes to the advancement of cleaner and more efficient aftertreatment technologies.

1.2.7 Motivation of this study

The literature review shows that although there are many studies on SCR systems, each one is conducted under specific assumptions and limitations. In particular, there is still a need for research on modeling and validating SCR performance for large-displacement heavy-duty engines. The motivation for this master’s thesis stems from this need.

The engine considered in this study is a large diesel engine with a 12.7 L displacement, designed to meet Euro VI emission standards. Under Euro VI, the average NO_x emissions of heavy-duty engines over the WHTC cycle must not exceed 0.46 g/kWh

[3]. Maintaining such a low average value over the entire WHTC, which includes varying load and speed conditions, is extremely challenging. This is because the WHTC cycle covers a wide operating range from low-load urban segments to full-load high-power conditions. Therefore, the SCR system must maintain high NO_x conversion efficiency even during difficult moments such as cold starts, low exhaust temperatures, and sudden load changes. The model to be developed in this study will be designed to predict the behavior of the 12.7 L engine-SCR system throughout the WHTC cycle. It is planned to validate the model using real engine test data so that its accuracy can be assessed under transient conditions.

Another key motivation is to investigate the relationship between SCR catalyst volume and system performance. For treating the high exhaust gas flow of a large engine, the catalyst volume (the amount of active catalyst) is a critical parameter. As catalyst volume increases, the residence time of the exhaust gas within the catalyst increases, providing more active surface area, which generally leads to better NO_x reduction performance [16]. However, increasing catalyst volume also brings limitations in terms of cost, weight, and packaging space. Therefore, selecting an optimal volume is essential. This thesis will run simulations on the model for different catalyst volume scenarios and compare changes in outputs such as NO_x conversion efficiency and AdBlue consumption. In particular, it will determine the minimum catalyst volume required to achieve the target NO_x reduction efficiency and the performance margin of the system under the Euro VI cycle at that volume.

Furthermore, the developed model and its results are expected to serve as guidance in preparing for future emission standards. Upcoming regulations such as Euro VII will further lower NO_x limits and introduce additional test conditions (e.g., low-temperature operation, more extensive RDE testing) [10]. In this regard, the findings obtained from model-based analysis of the 12.7 L diesel engine will provide important insights for both optimization under current Euro VI conditions and for design changes needed to meet stricter future standards. Validating the model under the WHTC cycle will help understand the effectiveness of the SCR system in real-use profiles. The model will also be kept flexible to allow its use in other cycles or operating points. As such, it can form a foundation for next steps, such as simulating real driving data or developing injection strategies.

In conclusion, the motivation for this study is to fill gaps in the literature by creating a comprehensive model of a large-displacement diesel engine and its SCR system, validating this model under strict emission cycles to demonstrate its reliability, and revealing the impact of critical parameters on system performance. In doing so, the study will contribute both to academic literature and to the development of a model-based approach that can be applied in industrial settings. The findings obtained in this context will be valuable for improving NO_x control in heavy-duty engines and for developing strategies to comply with upcoming emission regulations.

2. METHODOLOGY

This section presents the methodology followed in the scope of the study. First, the technical specifications of the test engine used and the applied experimental conditions are explained. Then, the structure of the simulation model developed in the MATLAB/Simulink environment is introduced in two main components. Finally, the validation of the simulation model through comparison with real engine test data and the rationale behind the chosen validation method are discussed.

2.1 Technical Specifications of the Test Engine and Muffler

The test engine used in this study is a 12.7-liter, heavy-duty, inline 6-cylinder diesel engine. This engine is designed to comply with Euro VI emission standards. It has a bore of 115 mm, a stroke of 144 mm, and a connecting rod length of 230 mm, with a compression ratio of 17:1. The large displacement and six-cylinder configuration provide the necessary power and torque for heavy-duty applications, while the Euro VI-compliant design, supported by an advanced aftertreatment emission control system (Figure 2.1), enables the engine to meet stringent emission limits. A diesel oxidation catalyst, a wall-flow diesel particulate filter, Cu-zeolite SCR catalysts and an ammonia-slip catalyst. Ford Trucks adopted this compact layout to minimize chassis package volume and to reduce thermal losses between bricks. During the experiments, both raw exhaust and post-SCR emission values were monitored.

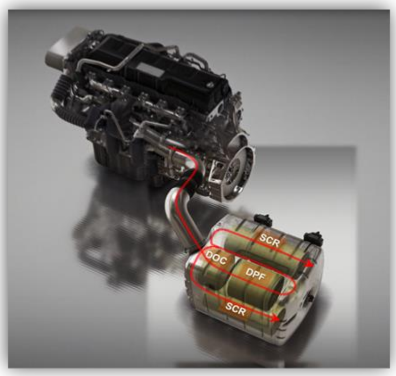

Figure 2.1 : Aftertreatment system.

2.2 Experimental Test Conditions

To evaluate the performance and emission characteristics of the engine, tests were conducted using an engine dynamometer. During testing, the World Harmonized Transient Cycle (WHTC), a globally standardized transient cycle for heavy-duty diesel engines, was applied. WHTC is a dynamic engine test cycle mandated under Euro VI emission certification and lasts for 1800 seconds [25]. It consists of variable engine speed and torque to represent real-world heavy-duty vehicle operating profiles and includes both cold and hot start phases. During the WHTC, the engine transitions through a wide range of operating points, from idle to full load, providing a comprehensive dataset for model validation.

In the dynamometer tests, engine performance parameters such as torque, speed, and fuel consumption were measured in real time, along with exhaust gas temperature and NO_x concentrations. NO_x levels before (engine-out) and after (tailpipe) the SCR system were recorded using appropriate analyzers. This allowed for monitoring both the internal engine performance and post-SCR emissions. The highly dynamic nature of WHTC offered a challenging yet comprehensive test environment to evaluate the model's behavior under transient conditions [26]. Consequently, it was possible to observe in detail whether the simulation model performed as expected under real-world driving conditions.

2.3 Simulation Model Structure

The developed model (Figure 2.2) was built in MATLAB/Simulink and is composed of two main components: (i) the SCR Control Model and (ii) the SCR efficiency calculation model. These two modules operate together by taking raw exhaust gas data from the engine as input, calculating the appropriate AdBlue dosage, and predicting the NO_x emissions after the catalyst. The model is designed to replicate both real-time control strategies and the physical dynamics of the system in an integrated manner.

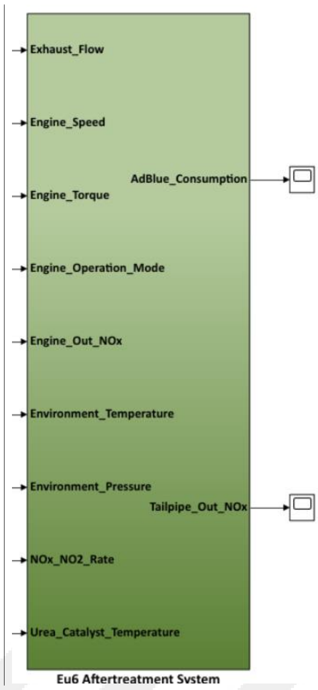

Figure 2.2 : Aftertreatment model inputs and outputs.

2.3.1 SCR control model

The SCR control model (Figure 2.3) includes control algorithms that calculate the required urea injection to reduce the NO_x emitted from the engine. This structure consists of the following sub-blocks:

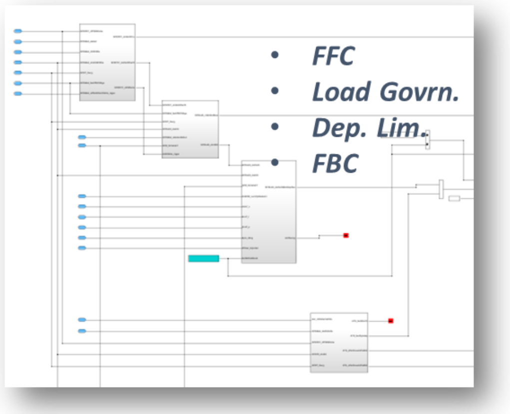

Figure 2.3 : SCR control model.

2.3.1.1 Feedforward control

Feedforward Control (FFC) block calculates the initial required urea dosing amount in advance based on engine operating conditions and the estimated engine-out NO_x production. FFC provides a rapid response by generating a dosing signal that matches the incoming NO_x flow to the SCR system.

2.3.1.2 NH_3 Load calculation

NH_3 Load calculation block, which is part of the SCR control strategy, performs a specific optimization operation on the dosing process based on the catalyst's current load capacity and operating conditions. Its primary role is to estimate the maximum permissible ammonia load that the catalyst can safely handle at a given time without leading to adverse effects such as ammonia slip or deposit formation. This estimation process takes into account several dynamic parameters, including: Catalyst temperature, current NH_3 storage level, Exhaust flow, catalyst aging condition. Based on these inputs, the NH_3 Load calculation block calculates a dynamic load limit, which reflects the catalyst's ability to convert NO_x with the available ammonia under current conditions. If the calculated ammonia dosing exceeds this limit, NH_3 Load calculation block reduces or postpones the injection amount to prevent NH_3 slip or saturation.

2.3.1.3 Urea deposit limitation

The urea deposit limitation is a crucial component in the control architecture of SCR systems, designed to prevent urea deposit formation under unfavorable operating conditions. Deposits typically form when the injected urea cannot fully vaporize and react due to suboptimal temperature or excessive dosing, especially during high-load transients or low-temperature start-up phases. In particular, the risk of deposit formation significantly increases when: Exhaust mass flow is high, accelerating transport and limiting residence time, exhaust gas temperature is in the critical window where thermolysis and hydrolysis of urea are incomplete, urea mass flow rate is too high for the catalyst or mixing section to handle effectively. To manage these risks, the urea deposit limitation continuously monitors real-time engine and exhaust conditions. It calculates a thermal and flow-based threshold for urea dosing and dynamically adjusts the injection rate to stay within this limit. If conditions indicate a high risk of deposit formation, the urea deposit limitation may: Reduce or delay urea injection, even if NO_x levels are elevated, track cumulative risk factors over time to estimate potential deposit accumulation, interact with other dosing limiters (e.g., NH_3 Load calculation block, NH_3 slip limiter) to maintain overall system balance. Some advanced implementations also include deposit modeling algorithms, which estimate the formation rate and mass of deposits based on operating history and enable preventive calibration or active purging strategies.

In summary, the urea deposit limitation ensures long-term reliability and performance of the SCR system by protecting the hardware from crystallization-related failures, especially under demanding transient and thermal boundary conditions.

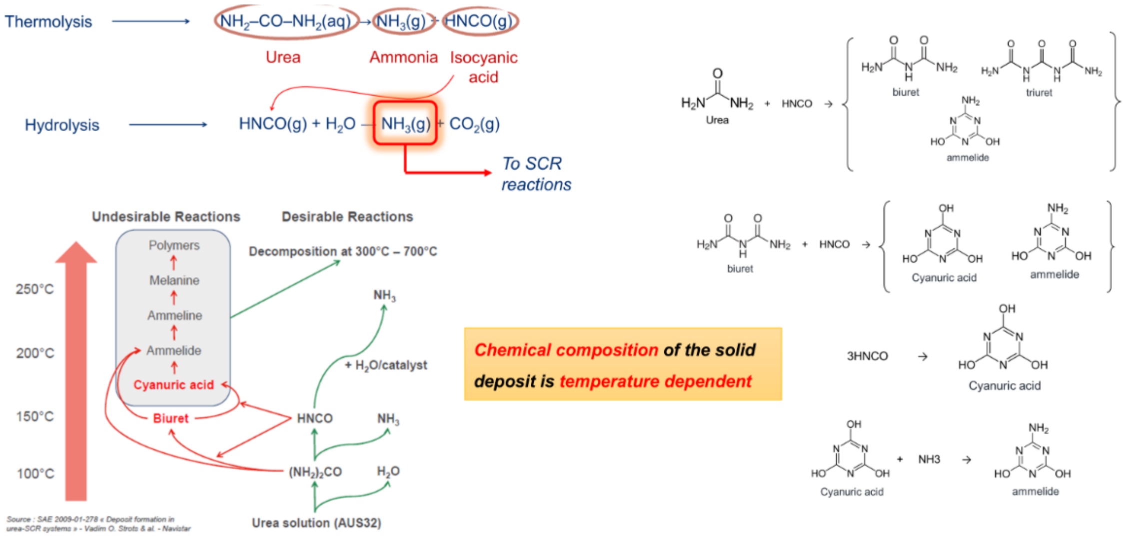

Figure 2.4 : Chemical reactions of urea deposit formation. Retrieved from [27].

2.3.1.4 Feedback control

Feedback Control (FBC) is a feedback mechanism that continuously adjusts the dosing signal based on the measured NO_x values at the SCR outlet. FBC corrects the output of FFC using feedback from the downstream NO_x sensor, ensuring that the target NO_x conversion efficiency is achieved and allowing the model to adapt to real system variations.

This control model is configured to emulate the urea dosing strategy of a real engine control unit (ECU) in software. The combination of feedforward and feedback control enables both fast response and precise long-term adjustment. Additional blocks such as load calculation and urea deposit limitation provide specific optimization and limitation functions, enhancing the stability and effectiveness of the dosing. As a result, the SCR control model determines the command (injection rate) to be sent to the urea injector based on real-time data from the engine.

2.3.2 SCR plant model

The SCR plant model simulates the dynamic behavior of the physical SCR unit and its associated components. This model (Figure 2.4) comprises two main subcomponents: the thermal model and the SCR efficiency calculation model.

2.3.2.1 Thermal model

The thermal model represents the temperature dynamics and thermal delays of the SCR catalyst. By using parameters such as exhaust gas flow rate, temperature, and catalyst mass, the model calculates how the temperature profile of the catalyst monolith evolves over time. This is especially critical for capturing the impact of catalyst temperature on NO_x reduction reactions during cold starts and load transitions.

2.3.2.2 Efficiency calculation model

The SCR efficiency calculation model estimates the NO_x conversion efficiency of the SCR catalyst. Taking into account factors such as input and output temperatures, exhaust mass flow, NO_x concentration upstream, the model predicts how much of the incoming NO_x can be converted into N_2 and H_2O at any given moment.

The urea injection command calculated by the SCR control model is fed as an input to the SCR system model. Based on this injection and the prevailing operating conditions, the SCR system model computes the TP NO_x emissions at the catalyst outlet.

In summary, the developed simulation model operates in an integrated manner to produce two key outputs: the AdBlue dosing rate and the TP NO_x value. The AdBlue dosing rate is the instantaneous injection amount determined by the control model (the actuator output of the model), while TP NO_x is the NO_x emission at the catalyst outlet predicted by the SCR efficiency calculation model. These outputs are then compared against experimental data for validation and evaluation purposes.

2.4 Model Validation

The reliability and accuracy of the developed model were comprehensively validated using real engine test data. Model validation was carried out by comparing the outputs of the simulation model with the data obtained from the WHTC dynamometer test, which is applied as part of the Euro VI certification process.Validation focused on four key performance parameters: Predicted NO_x conversion efficiency, SCR outlet NO_x emissions (TP NO_x), Feedforward controller signal (FFC), and AdBlue consumption. The outputs generated by the model were superimposed on the corresponding experimental measurements over the time axis and examined in detail. For each parameter, the extent to which the model curve followed the experimental data curve was graphically illustrated (see Figures 2.5-2.8). The results showed that the model was able to replicate the real system behavior with high accuracy across all critical parameters. Specifically, the relative error between model results and experimental data remained below 5% for each measured quantity. This 5% error margin indicates that the model has reached an acceptable level of accuracy, and the deviations in predicted values are within tolerable engineering limits.

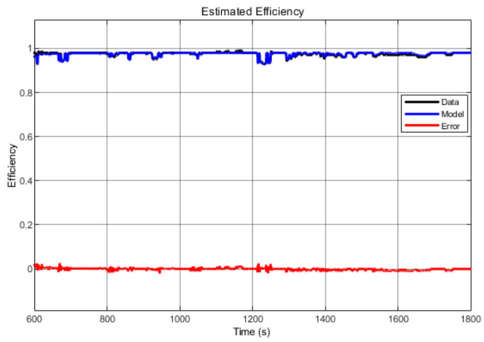

Figure 2.5 : Estimated NO_x conversion efficiency comparison**.**

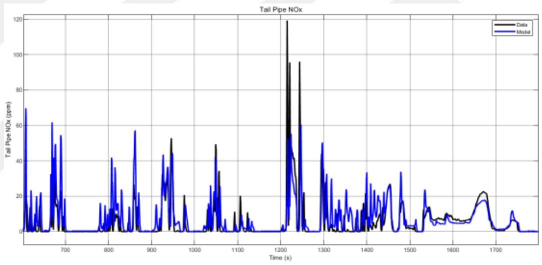

Figure 2.6 : Exhaust outlet NO_x comparison.

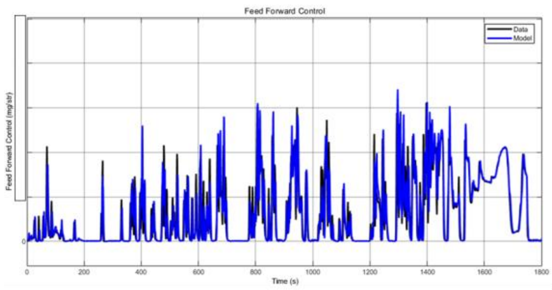

Figure 2.7 : Feedforward controller comparison.

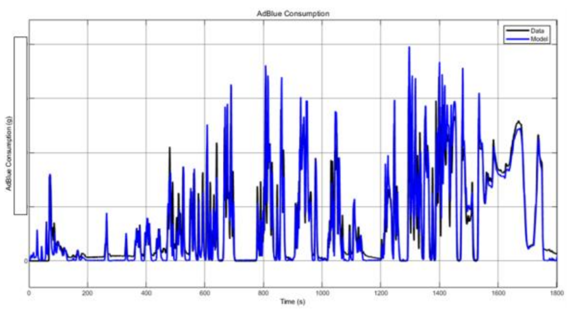

Figure 2.8 : AdBlue consumption comparison.

The validation results for each performance parameter can be summarized as follows: The NO_x conversion efficiency predicted by the model closely matched the actual efficiency curve calculated from dynamometer test data. As shown in Figure 2.5, the model output remained highly consistent with the measurements across the entire operating range, with no significant deviations observed.

Secondly, tailpipe (TP) NO_x values were evaluated. The comparison shown in Figure 2.6 indicates that the NO_x emissions predicted by the model followed the measured NO_x curve with an error margin of 3.2%. Notably, the model successfully captured both the accumulation and reduction of NO_x during transient phases, indicating its reliability under dynamic conditions.

Third, the Feedforward Control (FFC) signal was examined. The signal generated by the FFC block in the model was consistent with the feedforward urea injection strategy applied by the ECU in the experimental setup. As illustrated in Figure 2.7, the FFC signal was accurately implemented and matched the real system behavior with less than 1% deviation.

Finally, the model's prediction of AdBlue consumption was compared with experimental data. As shown in Figure 2.8, there was a strong correlation between the total urea consumption calculated by the model and the actual recorded values, with a 2.3% cumulative error. This confirms that the dosing strategy implemented in the model realistically reflects the behavior of the real system.

Overall, these results demonstrate that the model possesses a high predictive capability for both engine performance and emissions control under transient operating conditions.Selection of validation method

The reason for selecting a demanding and complex cycle like the WHTC for model validation is to test the model's performance under a scenario that closely resembles real-world driving conditions. Due to its sudden speed and load changes, the WHTC offers an ideal platform to evaluate the dynamic response of the model. The literature indicates that detailed models are often validated using simpler or steady-state tests, and the use of a complex cycle such as the WHTC is relatively rare [26]. In this study, the WHTC was intentionally used to achieve the desired level of accuracy and confidence, demonstrating that the model can represent the operating conditions required by Euro VI regulations.

The main validation approach involves assessing whether the difference between the model outputs and experimental data stays within a predetermined error margin. For this purpose, both average and instantaneous error percentages were calculated for each parameter, and deviations at critical points were analyzed. The 5% error threshold adopted here is considered a strict criterion for such a complex and transient simulation, providing a strong assurance of the model's reliability. This criterion confirms that the model results are consistent enough for practical use. In conclusion, the validation technique employed, time-based comparison using dynamic cycle data, combined with the 5% error margin, demonstrates that the model accurately captures overall trends and produces quantitatively precise predictions. This approach is critically important for establishing a reliable simulation platform within the model-based development process.

3. ANALYSES

This section presents parametric analyses focused on the critical design parameters of the SCR system. The analyses are based on the findings of the study titled "Hardware and Software Optimization of SCR Systems in Internal Combustion Engines" as well as technical simulations conducted within this work. The aim is to investigate the effects of various parameter values on the performance of the SCR (Selective Catalytic Reduction) system and to inform system design decisions. In this context, each parameter was varied by specific proportions, and the resulting outcomes were interpreted with accompanying graphical representations.

3.1 Parameters and Simulation Matris

Three main design parameters were addressed in the parametric analyses. Each parameter was varied within defined ranges to observe the system response: SCR catalyst volume: Scenarios where the reference volume was decreased by 40% and increased by 20%. Urea injector capacity: Scenarios where the injector’s dosing capacity was reduced by 20% and increased by 20%. Catalyst activity (aging effect): Scenarios simulating aged catalysts, with the NO_x conversion efficiency reduced by 10% and 20%. For each parameter, the above variations were applied and a simulation matrix was constructed. In the matrix, only one parameter was changed at a time while the others were held at their reference values. This approach enabled isolated, single-variable analyses to evaluate the impact of each factor on system performance. Including the reference (baseline) case, a total of seven simulations were conducted (one baseline and two variations for each parameter). The simulation matrix is summarized in Tables 3.1-3.3.

Table 3.1 : Effects of catalyst volume.

SCR Catalyst Volume (a)	Tail Pipe NOx (mg/kWh)	AdBlue Consumption (g)
1	128.9	X
0.6	325.9	X-0.7
1.2	128.9	X+0.5

Table 3.2 : Effects of urea injector capacity.

Urea injector capacity (a)	Tail Pipe NOx (mg/kWh)	AdBlue Consumption (g)
1	128.9	X
0.8	129	X-1.1
1.2	128.9	X

Table 3.3 : Effects of SCR catalyst efficiency.

SCR Catalyst Efficieny (a)	Tail Pipe NOx (mg/kWh)	AdBlue Consumption (g)
1	128.9	X
0.9	521.6	X+0.7
0.8	917.1	X+1

3.2 Performance Criteria

The results of each scenario were compared using key performance metrics that characterize SCR system performance. The evaluated performance indicators include: TP NO_x emissions (g/kWh): The final NO_x emission level at the SCR outlet. Expressed as the mass of NO_x per unit of work produced by the engine in grams per kilowatt-hour. This value reflects the overall NO_x reduction effectiveness of the SCR system. AdBlue consumption (g): The amount of urea solution (AdBlue) consumed during the test or over a specific cycle. It represents the total reductant usage and is an important metric linked to operating costs. These metrics helped quantify the impact of each parameter variation relative to the baseline scenario. In particular, TP NO_x emissions were closely analyzed, as they are critical indicators of compliance with emissions regulations. Meanwhile, AdBlue consumption provided insight into the system's operational demands. The effects of each parameter variation on these performance metrics are discussed in the following subsections.

3.2.1 Effects of SCR catalyst volume

The SCR catalyst volume is one of the most critical physical parameters determining the NO_x reduction capacity of the system. Increasing the catalyst volume provides more reaction space and residence time for the exhaust gas, potentially improving NO_x conversion efficiency. Conversely, reducing the volume increases gas flow velocity and shortens contact time, resulting in lower conversion efficiency [12].In this study, two scenarios were examined in which the catalyst volume was 40% smaller and 20% larger than the baseline value.

A 40% reduction in volume caused a dramatic increase in TP NO_x emissions. According to simulation results, this significant volume reduction led to approximately a threefold increase in tailpipe NO_x emissions. In other words, if the TP NO_x emission in the baseline case was X mg/kWh, it rose to ~3X when the volume was reduced (Table 3.1). This result can be explained by increased gas velocity and decreased residence time in the smaller catalyst, which prevents sufficient NO_x conversion. Additionally, even when the desired NH_3/NO_x ratio is achieved, the lack of adequate active surface area results in incomplete reduction reactions and a loss of efficiency.

In the scenario where catalyst volume was increased by 20%, only a modest improvement in TP NO_x emissions was observed (Table 3.1). Although enlarging the catalyst by one-fifth of the baseline volume led to a slight increase in NO_x conversion efficiency, this improvement was not as pronounced as the performance drop in the first scenario. The TP NO_x value decreased only slightly compared to the baseline. This limited benefit is attributed to the baseline design already being optimized, making additional volume yield diminishing returns: while extra volume theoretically enhances conversion efficiency, the practical gain remains limited in an already efficient system. Still, increased volume can improve ammonia storage capacity and help mitigate NO_x spikes during transient conditions, though this simulation was conducted under steady-state conditions, limiting the impact.

Overall, catalyst volume analyses reveal that the NO_x control performance of an SCR system is highly sensitive to catalyst size. Volume reduction leads to unacceptable emission increases, while moderate increases can provide incremental improvements. From a design perspective, including a safety margin in catalyst sizing (e.g., slightly exceeding the calculated minimum volume) appears critical to ensuring compliance with NO_x emission limits. Otherwise, the catalyst may be undersized during high engine load conditions, leading to regulation violations.

3.2.2 Effects of urea injector capacity

The AdBlue injection system used in the SCR system is responsible for delivering an appropriate amount of urea solution based on the NO_x levels at the engine outlet. The injector's maximum dosing capacity is a critical limit, particularly under high engine load or elevated NO_x production, to ensure sufficient ammonia supply. Therefore, reducing the injector capacity is expected to negatively affect NO_x conversion, while increasing it may improve system flexibility.

In the simulations, the injector's maximum flow capacity was reduced and increased by 20% relative to the baseline. Reducing the capacity by 20% prevented the SCR system from delivering the required amount of ammonia in demanding conditions. In this scenario, total AdBlue consumption showed a slight decrease compared to the baseline (Table 3.2). This reduction was due to the injector's physical limitation, which restricted urea injection at certain operating points below the desired levels. However, insufficient urea injection directly translates to a portion of NO_x escaping untreated. Indeed, simulation results confirmed that reducing injector capacity led to increased tailpipe NO_x emissions compared to the baseline (Table 3.2). Although this increase was not as drastic as in the reduced catalyst volume scenario, it was still significant. Especially at high-load operating points where the injector operated near 100% duty, NO_x conversion efficiency dropped, resulting in higher tailpipe NO_x. Therefore, if the injector is undersized, the SCR system cannot operate at full potential; even a small ammonia dosing shortfall can cause disproportionately high NO_x slip.

Conversely, increasing injector capacity by 20% did not yield a notable change in performance metrics. AdBlue consumption remained almost the same as in the baseline, and no significant improvement was observed in TP NO_x emissions. This suggests that the baseline injector already had sufficient capacity, and the additional 20% margin was not utilized under normal operating conditions. In other words, the current control strategy already provides adequate NO_x conversion using the baseline injector, and extra maximum flow capacity was unnecessary. Still, the added capacity may offer a safety margin during transient operations or unexpected NO_x spikes. Given that this simulation was conducted under steady-state conditions, the lack of observable benefit from the increased capacity is understandable.

In conclusion, the injector capacity analysis shows that proper sizing of the SCR dosing system is critical but exceeding the optimal capacity offers no additional benefit. Undersized injectors compromise NO_x control, while oversized injectors do not further reduce emissions (as dosing is already near the stoichiometric ratio under control logic). Therefore, during design, the injector must be sized to handle peak NO_x output from the engine, while recognizing that excessive capacity brings no advantage and may pose a risk of deposit formation. The issue of deposit risk will be examined in the following sections.

3.2.3 Effects of catalyst efficiency loss (aging)

SCR catalysts gradually lose activity over their service life due to factors such as thermal aging, poisoning, and soot accumulation. This degradation reduces the effective surface area and reactivity of the active sites, leading to a lower NO_x conversion rate at a given temperature and ammonia dosing compared to a fresh catalyst [16]. In real-world applications, the efficiency of SCR catalysts can significantly decline near the end of their life. Different types of SCR catalysts (Cu, Fe, V) with different efficiency can also be used for different regulation levels. To examine this effect, the chemical reaction efficiency (activity) of the catalyst was reduced by 10% and 20% relative to the reference condition in the simulation environment.

A 10% reduction in catalyst efficiency resulted in a noticeable increase in TP NO_x emissions. With a catalyst operating at 10% lower efficiency, the tailpipe NO_x reached 521.6 mg/kWh (approximately 0.522 g/kWh), which is a significant rise compared to the reference case (Table 3.3). When the efficiency dropped by 20%, TP NO_x emissions rose even more dramatically to 917.1 mg/kWh (0.917 g/kWh) (Table 3.3). These results demonstrate that even a seemingly modest reduction in catalyst activity can exponentially increase NO_x emissions. The 20% aging scenario almost halved the NO_x control capacity of the system, pushing emissions to unacceptable levels.

Notably, the decrease in catalyst efficiency did not directly affect AdBlue consumption, since the urea dosing strategy in the simulation is based on engine-out NO_x levels, the amount of urea injected remained nearly constant despite catalyst aging. However, the effectiveness of this dosing was reduced due to the lower catalytic activity, meaning less NO_x was converted for the same amount of injected AdBlue. This implies a decrease in NH_3 utilization efficiency with catalyst aging. In other words, while each unit of NH_3 converts more NO_x in a fresh catalyst, the same amount in an aged catalyst results in less NO_x reduction. This can lead to an increased risk of ammonia slip (unreacted NH_3 emission), as the aged catalyst may not be able to react with all the injected NH_3.

These findings clearly highlight the strong negative impact of catalyst aging on SCR performance. During design and calibration phases, it is essential to account for the fact that catalyst efficiency will decline over time. The system must initially be designed with a performance buffer so that even when the catalyst ages, NO_x emissions remain within legal limits. This can be achieved either by designing a system with higher initial conversion efficiency (e.g., using a larger or more active catalyst) or by planning to increase dosing strategies and schedule catalyst replacement as it ages. The results show that even a 10% efficiency loss can lead to significant emission increases, making it critical to incorporate this durability factor into SCR system planning.

3.3 Impacts on Design Decisions and Sensitivity Analysis Results

Based on the detailed findings from the parametric analyses presented above, the following key conclusions and recommendations have been drawn regarding SCR system design and optimization.

Catalyst volume was identified as one of the most influential physical parameters affecting overall system performance. A 40% reduction in volume led to a multiple-fold increase in NO_x emissions, completely undermining emissions compliance. Therefore, ensuring a sufficiently sized catalyst is critical in design. To meet emissions targets, the catalyst volume should be designed above the calculated minimum threshold, even if packaging or design constraints exist. Conversely, moderate increases in volume yielded only marginal gains due to diminishing returns, indicating that oversizing the catalyst may not be economically or spatially efficient.

In the analyzed range (±20%), injector capacity had a less dramatic effect on system behavior than catalyst volume or efficiency. As long as the injector can supply the necessary urea under demanding conditions, performance is maintained. Increasing the capacity beyond this point provided no additional benefit under normal operation. This suggests that the current injector sizing is already optimal. However, designers must ensure that the injector can meet the engine's worst-case NO_x production rate. Insufficient capacity at full load, for instance, would compromise NO_x reduction. Literature also confirms that underdosing leads to unconverted NO_x emissions. Thus, injector sizing should be treated as a reliability factor, oversizing offers little advantage and may even increase deposit formation risks.

System performance was found to be highly sensitive to reductions in catalyst activity. A 10-20% decrease in effectiveness significantly increased TP NO_x emissions. These findings highlight the need to account for catalyst aging in long-term system design. Designers must either build in sufficient overcapacity in the initial design or plan for catalyst regeneration or replacement after certain operating hours. Sensitivity analysis revealed that changes in catalyst activity had a strong, nonlinear effect on NO_x emissions, indicating that emissions control strategies must be flexible enough to adapt to aging effects (e.g., with adaptive dosing algorithms, though these have limits).

These parametric analyses clearly reveal the most critical SCR design parameters and their impact boundaries. Catalyst volume and activity are primary determinants of emissions performance. Injector dosing system capacity becomes a secondary concern once minimum requirements are met. This highlights the need for a balanced optimization approach in both hardware (e.g., catalyst sizing, material) and software/calibration (e.g., dosing strategies). Sensitivity analysis has provided design engineers with quantitative insights into acceptable variation ranges and parameters requiring zero tolerance for error. Consequently, both the minimum design requirements and priority areas for improvement have been identified. Applying this type of parametric evaluation in the design phase contributes to the development of more reliable and efficient SCR systems.

These present graphical summaries of the effects of parameter variations (catalyst volume, injector capacity, and catalyst activity) on TP NO_x emissions, AdBlue consumption, and NO_x conversion efficiency. The trends in the figures align with the conclusions discussed above.

4. DISCUSSION

This section discusses the findings obtained from the simulation and parametric analysis of the SCR system developed for a heavy-duty diesel engine. The aim is to interpret the results in the context of system performance, evaluate the impact of key design and calibration parameters, and provide engineering insights into the optimization of SCR systems under real-world operating conditions.

4.1 Hardware Cost

Simulation results of the SCR system demonstrate that increasing catalyst volume improves NO_x conversion efficiency up to a certain point, but this improvement diminishes beyond a threshold. As emphasized in the literature, "the NO_x removal efficiency increases with decreasing space velocity (increasing catalyst volume) for a given flue gas flow rate"[16]. However, excessive catalyst volume yields diminishing returns in NO_x reduction while significantly increasing cost. Indeed, as catalyst size grows, the amount of active material required rises proportionally, resulting in a linear increase in cost. According to EPA data, catalyst prices were reported to be in the range of $5,000-6,000 per cubic meter in 2011[16], indicating that any increase in volume directly burdens the budget.

Conversely, drastically reducing catalyst volume severely degrades NO_x conversion efficiency, leading to undesirable outcomes. Simulations show that using a smaller catalyst shortens the exhaust gas residence time within the catalyst, causing a sharp increase in NO_x emissions. The results reveal that total NO_x emissions exceed regulatory limits. Considering the Euro VI heavy-duty engine NO_x limit of 0.4 g/kWh [3], it is clear that undersizing the catalyst can easily breach this threshold. This underscores the fact that there is a regulatory lower bound on catalyst volume, below which compliance is not possible.

Therefore, determining the minimum effective catalyst volume is of critical importance. An optimal catalyst size that both satisfies emissions standards and minimizes cost provides an economically sound solution for SCR system design optimization.

4.2 Aging Durability

The modeling studies conducted clearly demonstrate the significant impact of SCR catalyst aging on system performance. Reductions in catalyst efficiency by 10% and 20% (due to thermal aging or poisoning, for instance) were shown to cause a dramatic increase in total NO_x emissions. In the simulations, these increases led to TP NO_x levels exceeding regulatory limits. Indeed, vehicles equipped with aged or degraded SCR systems can emit NO_x far above legislative thresholds [10]. This finding highlights how sensitive SCR systems are to the effects of aging.

Catalyst aging results in a reduction of active surface area and catalytic activity over time. Consequently, after a certain period of use, the catalyst may require regeneration, cleaning, or replacement [16]. Literature reports indicate that factors such as hydrothermal aging, sulfur accumulation, phosphorus and metal poisoning significantly reduce the efficiency of various SCR catalysts, including copper- and iron-based zeolites [10]. Therefore, it is essential to account for aging effects during SCR system design and calibration. For instance, a system that comfortably meets emission targets when new may exceed regulatory limits once catalyst efficiency drops by 20%. This necessitates designing and calibrating the system with a safety margin that accommodates expected degradation.

Furthermore, monitoring and control strategies should be implemented to detect and compensate for loss in conversion efficiency over time, such as adaptive dosing control or periodic maintenance alerts. Ultimately, enhancing catalyst durability and taking proactive measures against aging are critical to ensure that NO_x emissions remain within legal limits throughout the vehicle’s service life.

4.3 Calibration Adjustments

Simulation studies also examined the impact of changes in SCR injector capacity (AdBlue dosing system capacity) on emission performance and reductant consumption. The results revealed that increasing the injector capacity provided limited benefit in reducing NO_x emissions but significantly affected AdBlue consumption. A high-capacity dosing system may allow urea injection beyond what is necessary; in such cases, while NO_x emissions do not improve further, consumption increases and potential risks emerge. Specifically, excessive ammonia injection may lead to ammonia slip, where unused ammonia passes through the SCR catalyst unreacted, resulting in undesirable environmental and hardware outcomes [28]. Conversely, an under-sized injector may fail to meet the required ammonia levels under high engine load conditions. In such cases, insufficient dosing leads to a drop in NO_x conversion efficiency, making emissions control more difficult near regulatory thresholds [28]. Therefore, dosing calibration must strike a precise balance: underdosing results in "a fraction of NO_x that otherwise could be reduced will remain unconverted" [28], while overdosing fails to further reduce emissions and risks ammonia slip or deposit formation.

Calibration strategies must both ensure compliance with NO_x regulations and guarantee efficient use of the reductant. Ideally, the injected ammonia should match the inlet NO_x amount in a stoichiometric ratio ($NH_3/NO_x \approx 1$) with effective mixing. Theoretically, an $\alpha = 1$ dosing ratio offers 100% NO_x reduction potential, and in practice, this can yield around 90% NO_x conversion efficiency with <20 ppm ammonia slip [29]. Thus, control algorithms should dynamically optimize injection rates by considering real-time engine-out NO_x and stored ammonia levels in the catalyst. Additionally, literature reports note that overdosing can cause catalyst deposits and sensor poisoning, prompting manufacturers to define dosing limits to minimize ammonia slip risk [28]. In conclusion, SCR system calibration must optimize both emission performance and reductant consumption. This optimization should aim to achieve minimal AdBlue usage and safe operating conditions without exceeding emission thresholds under various engine loads.

4.4 General Evaluation

The conducted study has demonstrated that the Model-Based Development (MBD) approach offers significant advantages for optimizing SCR (Selective Catalytic Reduction) systems. By utilizing simulation models, hardware selection and calibration strategies can be extensively evaluated in a virtual environment before physical prototypes are built. This approach allows for rapid testing of various catalyst volumes, injector capacities, or control algorithms, enabling a balanced trade-off between cost and performance. The literature also supports that optimization studies aiming to minimize fuel and urea consumption while maintaining NO_x and NH_3 emissions within Euro VI limits have yielded successful results [7]. For instance, in a study using model-based optimization, peak NH_3 slip in the WHTC test cycle was reduced from 102 ppm to 47 ppm, and fuel consumption improved by 1.5% compared to conservative calibration [7]. These results highlight how virtual calibration improvements through MBD enhance emission performance and operational efficiency.

Compared to traditional experimental methods, the model-based design and validation process offers considerable advantages. Virtual development enables rapid analysis of numerous scenarios within the parameter space, allowing physical testing only for the most promising solutions. This significantly reduces both the time and cost of the overall development process [30]. Indeed, the assessment that “virtual powertrain calibration can considerably reduce time and cost of product development process while increasing the product quality” [30] succinctly summarizes the motivation behind the industry's adoption of the MBD approach. Furthermore, with MBD, system behavior can be validated and requirements can be verified early in the design phase, preventing late-stage design errors or deficiencies. This minimizes the need for experimental rework cycles and prototype revisions, making the product development process more efficient.

In conclusion, the model-based development approach has enabled a comprehensive optimization of both hardware and software components of the SCR system. As a result, it has facilitated compliance with emission regulations while ensuring a cost-effective and reliable design.

5. CONCLUSION AND FUTURE WORK

This section presents the overall conclusions derived from the modeling and simulation work on the SCR system developed for a heavy-duty diesel engine. The key findings from validation and parametric analysis are summarized, and the implications for system design and calibration are discussed. In addition to summarizing the key findings of this study, this section also outlines future research opportunities identified throughout the work. These include the integration of advanced control strategies, exploration of dual-dosing SCR architectures, development of catalyst aging and durability models, full engine-aftertreatment co-simulations, and improved calibration techniques for deposit prediction, each offering potential to enhance the robustness, applicability, and long-term accuracy of SCR system simulations.

This thesis presented the development and validation of a detailed Selective Catalytic Reduction (SCR) system model for a 12.7-liter Euro VI diesel engine using MATLAB/Simulink. The model was validated against World Harmonized Transient Cycle (WHTC) engine dynamometer data, a 1800-second transient test used for Euro VI certification. The close agreement between simulated and measured NO_x reduction over the WHTC confirms that the model accurately captures the SCR catalyst dynamics under real-world transient operating conditions. This high-fidelity validation provides confidence that the model can reliably predict tailpipe emissions and reductant (AdBlue) consumption for various scenarios, making it a valuable tool for development.

Parametric simulation studies were then conducted to assess the influence of key SCR design and operating parameters - namely catalyst volume, urea injector capacity, and catalyst efficiency (aging) - on tailpipe NO_x emissions and AdBlue usage. SCR catalyst volume was found to have a pronounced effect on NO_x conversion efficiency. Increasing the catalyst volume significantly enhanced NO_x reduction, as the larger volume provides more active surface area and longer residence time for ammonia-NO_x reactions to occur. This led to lower tailpipe NO_x emissions for a given dosing strategy.

However, the results also showed diminishing returns beyond a certain catalyst size - once the catalyst volume is sufficiently large to achieve >90% NO_x conversion, additional volume yields only marginal gains in emission reduction. This implies that an optimal catalyst size can be identified where Euro VI emission targets are met without unnecessary extra catalyst (and thus avoiding added cost and weight). An appropriately sized SCR catalyst can therefore minimize NO_x output while keeping AdBlue consumption efficient, whereas an undersized catalyst would struggle to meet emissions limits even with aggressive dosing. Notably, simply increasing catalyst volume (or dosing) to push conversion higher must be balanced against the risk of ammonia slip - injecting excessive reductant beyond the catalyst's capacity for reaction results in NH_3 passing through unreacted. The modeling results underscored this trade-off, reinforcing the need for balanced SCR sizing and dosing strategies to maximize NO_x conversion without incurring NH_3 slip.

The urea injector capacity was similarly shown to be a critical design parameter for SCR performance. Simulation of various injector flow-rate capacities revealed that an undersized urea injector can become a bottleneck during high engine load and speed conditions in the WHTC. In those transient peaks, engine-out NO_x generation is high, and if the injector cannot supply the required amount of urea (ammonia) quickly enough, the SCR catalyst becomes ammonia-limited. This leads to temporary NO_x breakthrough events where tailpipe emissions spike above the target. The study found that ensuring sufficient injector capacity to meet peak dosing demand is essential for maintaining low NO_x emissions throughout transient operation. When the injector was upsized to provide the necessary dosing rate even under worst-case conditions, the SCR system consistently achieved the desired NO_x conversion with no breakthrough. On the other hand, once the injector capacity exceeded the needed threshold, further increasing it had little to no impact on tailpipe emissions - an oversized injector offers no additional benefit if it already can deliver the maximum required AdBlue flow. This result highlights that there is an optimal injector specification: it must be just large enough to handle peak NO_x events, but oversizing beyond that point only adds cost without improving performance. Importantly, while injector capacity sets the upper limit for dosing, the total AdBlue consumption over a cycle is dictated by the control strategy and demand - the model indicated that providing a higher capacity does not increase AdBlue usage by itself, it simply provides headroom so that the dosing system can supply what is needed when it is needed. In summary, the SCR system must be equipped with an injector capable of meeting peak transient demands to avoid NO_x slip, but excessive injector capacity is unnecessary once that criterion is met.

Catalyst efficiency, or aging state, was another key factor analyzed, representing the loss of catalytic activity over time due to thermal aging or poisoning. The simulations showed that catalyst aging can have a significant adverse impact on SCR performance. As the catalyst becomes aged and its active sites or overall efficiency are reduced, the NO_x conversion rate drops, resulting in higher tailpipe NO_x for the same operating conditions and dosing strategy. Even a moderate reduction in catalyst efficiency led to noticeable increases in NO_x emissions in the model, indicating a reduced margin for compliance as the system ages. To compensate for an aged catalyst, the control system would need to inject more urea to achieve the same level of NO_x reduction - however, there are practical limits to this compensation because of the aforementioned ammonia slip constraint and the kinetics of the reactions. The study's findings suggest that a catalyst with, for example, 20% lower efficiency (due to aging) might require significantly more AdBlue and still might not fully reach the original NO_x performance, especially during fast transients when reaction kinetics are already challenged. This underscores the importance of accounting for aging in the design and calibration: SCR systems should be designed with enough initial conversion capacity (or additional features like larger volume or dual dosing) to meet emission standards not just when new, but also at end-of-life conditions. The model, being a calibrated first-principles representation, proved useful in simulating these what-if aging scenarios. It provides insight into how quickly performance could degrade and helps in formulating strategies (such as more conservative NO_x setpoints or adaptive dosing control) to ensure compliance throughout the vehicle's lifetime. In summary, catalyst degradation was observed to raise NO_x emissions and potentially increase urea consumption, highlighting a need for robust control strategies and possible design margins to mitigate aging effects.

Overall, the key outcomes of this work demonstrate how model-based development (MBD) can substantially aid in optimizing SCR system performance while minimizing development cost and effort. By using a high-fidelity Simulink model as a virtual testbed, we were able to pre-evaluate hardware configurations and calibration strategies in software, rather than relying solely on physical prototyping. For instance, the model allowed exploration of a range of catalyst sizes and injector capacities to find an optimal balance, something that would be costly and time-consuming if attempted through repeated hardware iterations. This approach capitalizes on the strengths of MBD: reducing the need for numerous physical prototypes and experiments, and thus saving cost and time. It also enables testing scenarios that might be impractical on an engine testbed (such as simulating an aged catalyst or extreme dosing strategies) early in the development cycle. The validated SCR model developed in this thesis can serve as a powerful engineering tool for system optimization. Engineers can use it to virtually assess how changes in hardware (e.g. a larger catalyst or a higher-grade catalyst formulation) or in software calibration (e.g. altering the dosing control algorithm or setpoints) would impact emissions and AdBlue usage before implementing those changes on a real engine. This model-based optimization approach aligns with findings in literature where a combined engine-aftertreatment simulation was used to meet emissions targets at minimal fuel/urea cost [7]. In our case, the SCR model helps to identify trade-offs between NO_x reduction and reductant consumption, guiding calibrations that achieve compliance with the least amount of AdBlue. Moreover, by integrating this SCR model into a larger powertrain simulation, manufacturers can evaluate the complete system behavior and optimize the calibration holistically, balancing engine-out NO_x (via EGR or engine tuning) with SCR capability to minimize overall fuel penalty while meeting Euro VI standards [7]. In conclusion, this work’s contribution lies in delivering a validated SCR simulation model and using it to gain engineering insights that would be difficult or expensive to obtain experimentally. It illustrates that MBD, when applied to aftertreatment systems, can accelerate development, enhance understanding of system interactions, and ultimately lead to an optimized design that achieves stringent emissions performance at lower development cost and risk.

5.1 Future Work

Building on the successful development and application of the SCR system model, several avenues for future work are recommended to further improve and extend this research.

5.1.1 Advanced control strategies

Implement more complex real-time control algorithms for the SCR system to enhance performance under dynamic conditions. For example, a model-predictive control (MPC) approach or adaptive control scheme could be developed to modulate urea injection in a predictive manner. Such controllers can account for catalyst dynamics and upcoming engine conditions to minimize NO_x and NH_3 slip simultaneously. Prior studies have shown that MPC-based SCR control can significantly reduce ammonia slip and even improve fuel economy compared to static calibrations [7]. Developing and testing an MPC or similar advanced controller within the current model would demonstrate how much additional benefit can be gained in NO_x reduction and AdBlue efficiency through smarter control logic.

5.1.2 Dual dosing SCR system

Explore a twin-dosing SCR configuration in the model, where a second urea injector is added upstream in the exhaust (e.g. one injector positioned closer to the engine, in addition to the existing injector). Dual SCR dosing systems are an emerging technology to achieve ultra-low NO_x emissions (>98% reduction) under upcoming regulations. By injecting urea at two separate locations (one hotter, one cooler), a wider range of exhaust temperature conditions can be covered, improving NO_x conversion during cold-start and high-load transients. Incorporating this into the simulation would allow evaluation of the potential NO_x benefits and challenges (like control coordination and ammonia slip control) of dual dosing. The model could be used to experiment with injector placement, dosing split strategies, and the impact on transient emissions. Although dual SCR systems were not commonly used in heavy-duty trucks in 2022 [31], many manufacturers have recently started adopting this technology and publishing related studies. While this model does not yet include a dual dosing system, the integration of this technology into the simulation is planned for future work. Therefore, this study may provide a valuable foundation for the evaluation of dual SCR systems.

5.1.3 Catalyst aging and durability modelling

Integrate a detailed catalyst aging model into the SCR simulation to capture the gradual decline in performance over the catalyst’s lifetime. This would involve introducing empirically derived aging factors or kinetics (e.g. hydrothermal aging mechanisms that reduce active site availability over time) [32]. With an aging sub-model, one could simulate long-term usage scenarios, predicting how the SCR efficiency drops after several thousand hours of operation, and how that impacts emissions compliance. This extension would enable virtual durability testing: the model could help determine if the initial system design has enough margin to meet emissions at end-of-life, or if calibration adjustments (such as periodically increasing dosing or regenerating the catalyst) are needed. Incorporating aging effects also allows the development of adaptive control strategies that adjust dosing based on estimated catalyst health. Given that real SCR catalysts undergo degradation, adding this dimension to the model greatly increases its utility for life-cycle performance evaluation.

5.1.4 Full engine and aftertreatment co-simulation

Extend the modeling framework to include a full engine model and other aftertreatment components, enabling a complete engine-aftertreatment system simulation. Currently, the SCR model has been tested with recorded engine-out data; the next step is to couple it with a dynamic engine model (including combustion, turbocharging, EGR, etc.) and upstream devices like the diesel oxidation catalyst and diesel particulate filter. This holistic co-simulation would capture the interactions between engine calibration and SCR behaviour [7]. For instance, engine strategies that reduce engine-out NO_x (such as higher EGR rates or retarded fuel injection timing) can be evaluated alongside SCR efficiency and ammonia dosing requirements, to find an optimal balance that minimizes fuel penalty while still meeting NO_x targets. A full-system model would also allow testing of transient management strategies, like thermal management (exhaust temperature control to keep the SCR active) and ammonia slip mitigation via an ammonia slip catalyst if integrated. In essence, this future work would move towards a model-based calibration of the entire powertrain, where trade-offs between engine efficiency, fuel consumption, and aftertreatment performance are optimized in software. This approach is aligned with the industry trend of using simulation for system-level optimization to meet tightening emission standards at minimal cost.

In addition to the above key areas, other improvements can be envisioned. For example, enhancing the model fidelity by including urea injection physics in greater detail (such as droplet evaporation and spray dynamics) could improve accuracy in predicting NH_3 availability, especially during cold start. Another worthwhile direction could be real-time implementation of the model (or a simplified version) for Hardware-in-the-Loop (HIL) testing or as an onboard model for diagnostic or control purposes. Overall, the suggested future works aim to make the SCR model even more comprehensive and predictive, thereby extending its usefulness. By pursuing these enhancements, the model can evolve into an even more powerful tool for virtual development and optimization of diesel engine aftertreatment systems, helping manufacturers meet stringent emission targets with greater confidence and lower development costs. The continual tightening of NO_x regulations and the introduction of new technologies (like dual dosing and advanced catalysts) make such model-based investigations invaluable for staying ahead in clean engine development. Each proposed extension builds on this thesis's foundation, leveraging the proven SCR model to tackle broader challenges and ensure that model-based design remains at the core of efficient, innovative emissions control solutions for future diesel powertrains.

5.1.5 Deposit model calibration

This study which is already started on Ford Otosan, details an approach aimed at managing deposit accumulation within exhaust systems. Within the scope of the project, a specific number of vehicles were monitored under field conditions over a period of 10 days. During the monitoring period, operational data was collected from the vehicles at approximately 750-kilometer intervals. A critical component of the data collection process involved obtaining camera images illustrating the level of deposit accumulation inside the exhaust muffler.

The primary objective in collecting this real-world data is to enhance the accuracy of the existing particulate accumulation model and to facilitate its calibration. The calibration process involves matching the acquired operational data with camera images captured simultaneously, which depict the actual amount of accumulation. The amount of accumulation predicted by the model is compared against the actual amount observed in the images. Through these comparisons, areas where the model is not performing accurately or exhibits deviations are identified, and the model parameters are adjusted to correct these deviations. This iterative process of matching and parameter adjustment aims to enable the model to reliably estimate the amount of particulate accumulation in a vehicle based solely on its operational data.

Figure 5.1 presents a visual example of deposit accumulation, while Figure 5.2 illustrates a graphical model used to estimate the extent of such accumulation."

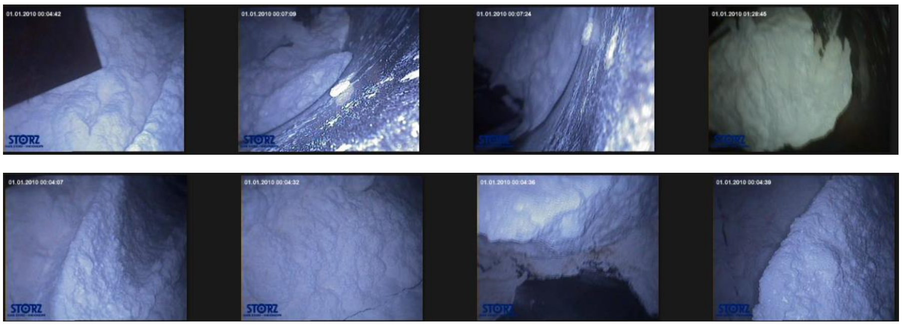

Figure 5.1 : Deposit image.

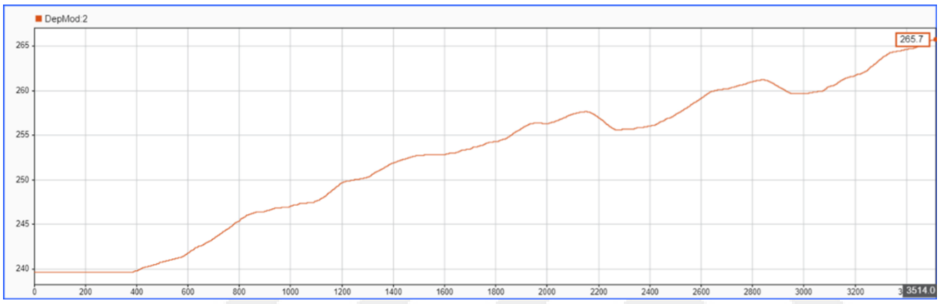

Figure 5.2 : Example of deposit model data (g).

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