

Master's Thesis in Automotive Engineering

1D Simulation Modeling for an Exhaust Aftertreatment System

SCR Calibration Modeling in GT-SUITE

Puneeth Ramanjaneyalu
September 2021

Division of Combustion and Propulsion Systems
Department of Mechanics and Maritime Sciences

CHALMERS UNIVERSITY OF TECHNOLOGY
Gothenburg, Sweden 2021
www.chalmers.se

Master's thesis in Automotive Engineering 2021

1D Simulation Modeling for an Exhaust Aftertreatment System

SCR Calibration Modeling in GT-SUITE

Puneeth Ramanjaneyalu



CHALMERS
UNIVERSITY OF TECHNOLOGY

Department of Automotive Engineering
Division of Combustion and Propulsion Systems
Chalmers University of Technology
Gothenburg, Sweden 2021

1D Simulation Modeling for an Exhaust Aftertreatment System
SCR Calibration Modeling in GT-SUITE
Puneeth Ramanjaneyalu

© Puneeth Ramanjaneyalu, 2021.

Industry Supervisor:Zemichael Yitbarek, Scania

Examiner and Academic Supervisor: Jonas Sjöblom
Professor at division of Combustion and Propulsion Systems
Mechanics and Maritime Sciences, Chalmers University of Technology.

Master's Thesis 2021
Division of Combustion and Propulsion Systems
Department of Mechanics and Maritime Sciences
Chalmers University of Technology
SE-412 96 Gothenburg
Telephone +46 31 772 1000

1D Simulation Modeling for an Exhaust Aftertreatment System
SCR Calibration Modeling in GT-SUITE
Puneeth Ramanjaneyalu
Department of Automotive Engineering
Chalmers University of Technology

Abstract

The Euro legislative regulations are imposed successively to hold back toxic elements that are harmful to the environment. Carbon monoxide (CO), hydrocarbons (HC) and nitric oxide (NO_x) are the major toxic elements that cause serious health hazards for the living species. From many research works, selective catalytic reduction (SCR) is the most promising technology to address NO_x. The objective of this project is to develop a surface reaction mechanism model, reaction rate calibration for SCR catalyst and validation.

Firstly, building the SCR catalyst and surface reaction mechanism model in GT-SUITE. The reaction rate calibration or characterization is performed for six reaction rate expressions with 18 unknown parameters by applying physical properties of the catalyst for example diameter and area of the catalyst. Furthermore, the digital laboratory Simulink black-box is utilized to produce the target reaction rate curves for all chemical reactions to calibrate the parameters then to compare with simulated GT-model results. Finally, validation for steady state or urea stairs, US, conditions and transient driving cycle conditions against WHTC (world harmonized transient driving cycles) for the Euro V regulations using tail pipe, engine-out emissions, mass flow rate and temperature traces experiments data.

Overall, chemical kinetics modeling for SCR catalyst in GT-SUITE was successfully implemented and have reasonable results for urea stair cases, but the outcome can be further improved for transient cycles by extract information from 3D CFD to 1D in the future. Inevitably, simulations analysis is the best possible way to validate the results in quick time with low cost and it is a key factor during the development process.

Keywords: SCR, catalyst, chemical kinetics, validation, modeling, simulations, calibration and experiment data.

Acknowledgements

First and foremost, I want to express my sincere gratitude to my supervisor Yitbarek Zemichael, NXPS, Scania who always gave me his full availability, constant support and guidance during the course of this project. This thesis would not have been possible without him.

I also want to thank my examiner and academic supervisor Jonas Sjöblom, Chalmers for his availability and valuable feedbacks during the course of the project.

Also, I feel proud to express my gratitude to Sabuco Pierre for the discussions throughout the project. I want to thank Suarez Andres for helping in solving technical problems and delivering simulink model for the project. Last but not least, big thanks to the whole NXPS team for the valuable feedback and support.

I want to give my endless gratitude to my parents. Thank you for always being there for me and supporting my decisions. I am forever grateful to all of you.

Puneeth Ramanjaneyalu, Gothenburg, September 2021.

Nomenclatures

$\mathbf{NH_3}$	Ammonia
$\mathbf{H_2O}$	Water
$\mathbf{O_2}$	Oxygen
Ze	Zeoliet
V	Vanadium
CO	Carbon Monoxide
$\mathbf{NO}_x$	Nitric Oxide
$\mathbf{CO(NH_2)_2}$	Urea
$\mathbf{CO_2}$	Carbon Dioxide
HC	Hydro Carbons
$\mathbf{N_2}$	Nitrogen
$\mathbf{NO_2}$	Nitrogen Dioxide
$\mathbf{NO}x$	Nitrogen Oxides
$\mathbf{NH_3}$	Ammonia
Cu	Copper
S	Surface Site
HNCO	Isocyanic Acid

Abbreviations

GT-SUITE	Gamma Technologies Engine Simulation Software
CFD	Computational Fluid Dynamics
SCR	Selective Catalytic Reduction
ASC	Ammonia Slip Catalyst
DPF	Diesel Particulate Filter
ANR	Ammonia to NOx Ratio
CPSI	Cells per Square Inch
WHTC	World Harmonized Test cycle

Contents

List of Figures **xiii**

List of Figures **xiii**

List of Tables **xv**

List of Tables **xv**

1 Introduction **1**
1.1 Europe Environmental Legislative Standards 1
1.2 Industry Background 3
1.3 Objective 4
1.4 Delimitations 4

2 Theoretical and Modeling Background **5**
2.1 Exhaust Aftertreatment System 5
2.2 Selective Catalytic Reduction (SCR) 6
2.3 Chemical Reaction Rate Equations 7
2.4 Simplex and Genetic Algorithm 8
2.5 Calibration Requirements 9

3 Methodology **11**
3.1 Building SCR Catalyst in GT-SUITE 11
3.2 Target Data from Simulink Black-box 12
3.2.1 Storage Target 13
3.2.2 Oxidation Target 13
3.2.3 DeNO$_x$ Standard Target 14
3.2.4 DeNO$_x$ Fast Target 14
3.2.5 DeNO$_x$ Slow Target 14
3.3 Calibration Process 14
3.3.1 Thermal Calibration 14
3.3.2 Storage Calibration (Adsorption Desorption) 15
3.3.3 Oxidation Reaction Rate Calibration 18
3.3.4 DeNO$_x$ Standard Reaction Rate Calibration 19
3.3.5 DeNO$_x$ Fast Reaction Rate Calibration 19
3.3.6 DeNO$_x$ Slow Reaction Rate Calibration 21

4 Validation **23**
4.1 Steady State or Urea Stairs Validation 24
4.1.1 Steady State Experiment 1: Low Mass Flow Rate 24
4.1.2 Steady State Experiment 2: Medium Mass Flow Rate 25
4.1.3 Steady State Experiment 3: High Mass Flow Rate 26
4.2 Transient State Validation 27
4.2.1 Ammonia NO_x ratio, ANR, 0.8 27
4.2.2 Ammonia NO_x ratio, ANR, 0.9 28
4.2.3 Ammonia NO_x ratio, ANR, 1.1 29
4.3 Source of error at high mass flow rates 29
4.3.1 Other factors for discrepancy between experiments and simulation results 30

5 Conclusion **31**

6 Future Work **33**

Bibliography **35**

7 Appendix **37**

List of Figures

1.1 NO_x with respect to successive legislation[1] 1
1.2 schematic representation of Euro VI heavy duty testing equipment system for emissions regulations[2] 2

2.1 Exhaust aftertreatment with split SCR 5
2.2 catalytic reduction 6
2.3 The requirements for the calibration process 9

3.1 project structure 11
3.2 SCR Catalyst in GT-SUITE 12
3.3 Simple representation of Simulink black-box model 13
3.4 Thermal calibration 15
3.5 SCR Catalyst in GT-SUITE 16
3.6 Ammonia Storage at 200°C 17
3.7 Ammonia Storage at 300°C 17
3.8 Ammonia Storage at 400°C 18
3.9 Ammonia Storage at 500°C 18
3.10 Oxidation outlet molefraction comparision 19
3.11 DeNO$_x$standard outlet NO conversion rate comparison 19
3.12 DeNO$_x$ fast outlet NO conversion rate comparision 20
3.13 DeNOx fast outlet NO_2 conversion rate comparision 20
3.14 DeNOx slow outlet NO_2 conversion rate comparision 21

4.1 GT-SUITE validation model 23
4.2 Low mass flow rate comparison 25
4.3 Medium range mass flow rate comparison 26
4.4 High range mass flow rate comparison 27
4.5 Ammonia NO_x ratio 0.8 28
4.6 Ammonia NO_x ratio 0.9 28
4.7 Ammonia NO_x ratio 1.1 29

List of Tables

1.1 Euro regulations I to VI for heavy duty diesel engines[3] 3

2.1 Reactions with parameters and targets 9

3.1 Inlet ammonia composition for all temperature ranges 13
3.2 Inlet composition in mole fraction for storage calibration 17
3.3 Inlet composition during oxidation reaction rate calibration 18
3.4 Inlet composition during standard reaction rate calibration 19
3.5 Inlet composition during fast reaction rate calibration 20
3.6 Inlet composition during slow reaction rate calibration 21

1
Introduction

With the clear evidence, the climb in the number of vehicle users rising now and then, there is always room for improvement in the developments of vehicle technology. The vast research and studies are still ongoing to optimize the engine and lower the emissions significantly worldwide. Since 1993 Euro regulations are successfully imposed, to control the emissions from vehicles that are immensely polluting the environment and causing serious health hazards. From the atmospheric studies, as the air pollution is significant especially from vehicles, this project makes a meaningful contribution to study the amount of harmful gas reduced from the engine before entering the atmosphere.

1.1 Europe Environmental Legislative Standards

The legislative standards are the law enforced by the legal act directives with in the Europe Union states. It is applicable for most of the land vehicles they are passenger cars, trucks, buses and two wheel vehicles. The emissions from heavy duty vehicles are increasingly stringent with respect to series of Euro regulation. From **Figure 1.1** the NO_x was significantly limited to 0.2g/kWh for Euro V which is 95% cut-down compared to Euro I.

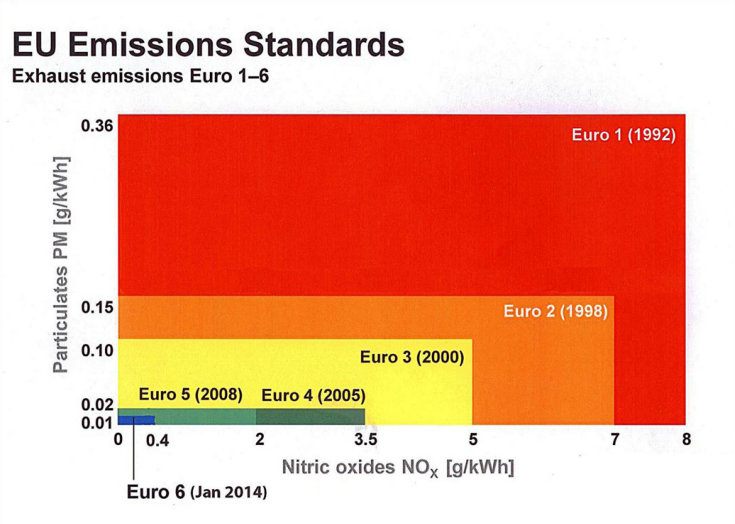


Figure 1.1: NO_x with respect to successive legislation[1]

However, it further leads to challenging investigations for the design of catalysts for the efficient aftertreatment systems for heavy duty vehicles. Ever since the Euro regulations are imposed to tighten the emissions for light and heavy-duty vehicles. It is a continuous effort and challenge to control the emissions coming out from the combustion engines, referring to the recent legislative emissions Euro VI for strengthening the emission standards for both particulate matter and nitrogen oxide (NO_x) were tightened by 90% compared to Euro III. The new techniques redeemed to ensure the predictions of toxic gases from the engine out. The method of real driving emissions (RDE) test comported for the Euro VI vehicles are shown in **Figure 1.2**. The testing equipment Semtech–recostar gas analyser that as flow meter to measure the exhaust gas flow rate and also has non-dispersive infrared (NDIR) detector to sense NO_x[2].

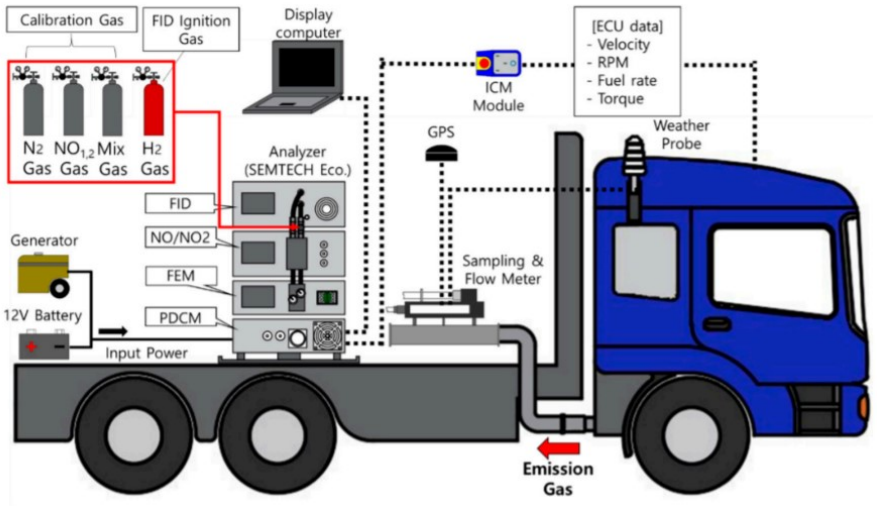


Figure 1.2: schematic representation of Euro VI heavy duty testing equipment system for emissions regulations[2]

The new era for emissions standards further to improve the air quality by introducing Euro VII standards for cars, buses and trucks. Association for emissions control by catalyst(AECC) propose principles to legislate actual tail pipe emissions to ensure health and well-being of everyone. Euro VII should also aim for application-neutral stringency, despite vehicle design and function. Moreover, it is important to implement new techniques of control strategy for the powertrain with out consumer market distortion. In fact, the introduction of new technologies required to achieve ultra-low pollutant emissions are close commercialization. Technologies such as cylinder deactivation, EGR cooler bypass and 48-volt systems could anable better engine out NO_x control, faster catalyst warm-up and thermal management strategies. Apparently, introduction of new technologies leads to increase in costs of meeting Euro VII standards rough estimations will be between €1500 and €4700 in 2025 and between €1400 and €4300 in 2030 therefore it will increase between 2% and 5% relatively to the current price [4]. For the heavy duty vehicles, steady state and transient conditions emission limits of NO_x, PM, CO and HC are described in **Table 1.1** from each successive regulation, it is clear that NO_x is reduced to 0.46g/kWh.

Table 1.1: Euro regulations I to VI for heavy duty diesel engines[3]

Emission Regulations	**Date**	**NO_x**	**PM**	**CO**	**HC**
Steady State		g/kWh	g/kWh	g/kWh	g/kWh
Euro I	1992	8	0.36	4.5	1.1
Euro II	*October* 1998	7	0.15	4	1.1
Euro III	*October* 2000	5	0.10	2.564	0.66
Euro IV	*October* 2005	3.5	0.02	1.5	0.46
Euro V	*October* 2008	3.5	0.02	1.5	0.46
Euro VI	*October* 2013	2	0.01	1.5	0.13
Transient Cycle	**Date**	g/kWh	g/kWh	g/kWh	g/kWh
Euro III	*October* 2000	5	0.16	5.45	-
Euro IV	*October* 2005	3.5	0.03	4	-
Euro V	*October* 2008	2	0.03	4	-
Euro VI	*January* 2013	0.46	0.01	4	-

1.2 Industry Background

Scania is continuously working on the developments of the engine evolution to mainly optimize the performance and lower the emissions significantly to give the top-class vehicle experience to the user worldwide. Primarily giving prominence to the living nature to promote the eco-friendly environment, this raises the anticipation to resolve harmful gases coming out from the engine. However, this project work will extend and continue their research work on the exhaust aftertreatment system with a 1D simulation modeling tool GT-SUITE, including surface chemical reactions modeling of selective catalytic reduction (SCR). Scania manufactures leading design and productive aftertreatment system technology, especially for freight heavy-duty trucks. Working continuously for more than a decade on the emissions control strategy in 3D CFD simulations and 1D simulations the company now extends the efforts to address the new Euro VI and Euro VII regulations to target the emissions analysis to achieve in 1D simulation modeling in GT-Power. Furthermore, the earlier projects carried out about the methodology to combine 3D CFD simulations with the chemical reactions needed to model the SCR which includes the NO_x conversion and ammonia slip analysis. However, this project further extends the attempt to calibrate or optimize the reaction rate parameters for SCR catalyst modeling. The advantage of trusting 1D simulations mainly because it is possible to extract for all the load points with respect to time where as in 3D CFD it is limited to low, medium and high load points. Even today many development engineers attempt to run hundreds of simulations to evaluate the closest possibilities to apply for real-time experimental rig testing applications. Hence, the simulation analysis give results in quick time with low cost and it is a key factor during the development process.

1.3 Objective

The primary objective of this project work includes establishing the streamlined workflow which would be used in the future for the aftertreatment system development technology.

- Develop a 1D simulation model for an exhaust aftertreatment system which includes the surface reaction mechanism models of SCR.
- Calibration in GT-SUITE and GT-Power.
- Documentation of the workflow and validation of the simulated results with engine out and tailpipe measurement data.

1.4 Delimitations

As the duration of the project is 20 weeks the scope of this project is as followed.

- The work is focused on building selective catalytic reduction (SCR) catalyst and surface reaction mechanism model.
- Producing experimental data setup from simulink black-box model.
- Characterization of unknown parameters for several reaction rate expressions to match with experimental data.
- The modeling and simulations are carried out in engine simulation tool Gamma Technology GT-SUITE and GT-power.

2

Theoretical and Modeling Background

2.1 Exhaust Aftertreatment System

Exhaust aftertreatment systems are necessary for the automotive powertrains to address exhaust emissions.The Euro regulations are getting tougher and tougher referring to the very recent regulation Euro VI of harmful gas NO_x, nitrogen monoxide (NO) and nitrogen dioxide (NO_2) is strictly prohibited from the vehicle manufacturers. Hence, this leads to investigate more closely to trace the problems. The adsorption and desorption of ammonia on the site elements strategy applied in this project to eliminate the amount of NO_x at the outlet successively.

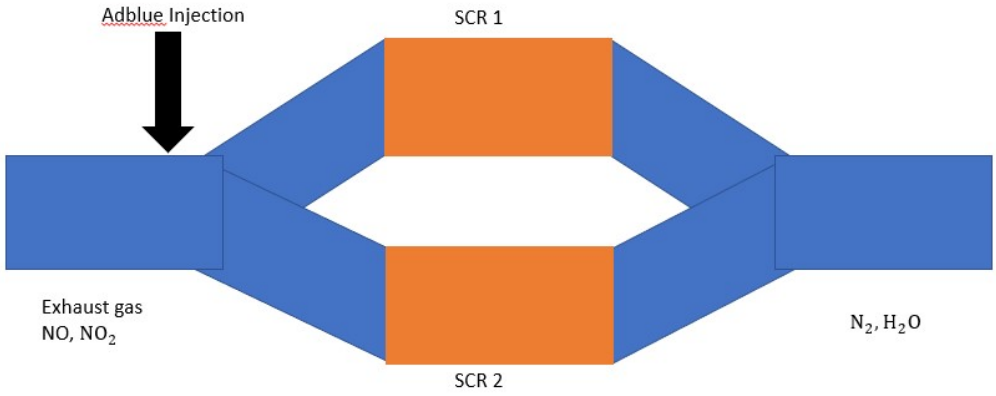


Figure 2.1: Exhaust aftertreatment with split SCR

The calibration is performed for the SCR vanadium catalyst. The exhaust gas along with toxic NO_x coming out from the engine are introduced through the SCR catalyst. From the external source adblue, typically 33% of urea and 67% of water solution injected just before the SCR [5]. The combination of chemical reactions takes place in the catalyst to reduce NO_x. The NO_x reacts with NH_3 with certain operating conditions to give out simple component N_2 and H_2O that are not harmful to the nature. The two split SCR catalysts with the same physical properties are used for Euro V experimental validation and the arrangement is shown in **Figure 2.1**. The experimental data particularly for WHTC driving cycle which is a legislative transient test cycle from the global technical regulation (GTR) for heavy vehicles

tests. The unreacted ammonia also called ammonia slip from the SCR are taken care by ammonia slip catalyst, ASC, has it is also dangerous if exposed to the environment.

2.2 Selective Catalytic Reduction (SCR)

The SCR technology was first applied in thermal power plants in Japan in the late 1970s and then slowly developed in Europe from the middle of 1980s, after a decade gradually it was popular in chemical processing industries[6]. Since 2005 urea-SCR technology was adopted in diesel engines, it is a form of converting the nitrogen oxides, NO_x referred as both NO and NO_2 into nitrogen, N_2 and water, H_2O with the aid of reducing agent for example, adblue or ammonia. Typically in the industries adblue is 33% of urea and 67% of water-diluted solution. The NO_x reduction with ammonia is mainly controlled by three important reactions usually standard, fast and slow SCR reactions. The ammonia is stored on the porous site elements for example vanadium coated on the substrate layer, after diffusion-reaction the toxic component denitrification to give a simple harmless products. In this project the method of global reaction kinetic model is developed to predict the amount of NO_x reduced at the catalyst outlet based on the experimental data sets. The detailed catalytic reduction is shown in the below **Figure 2.2**.

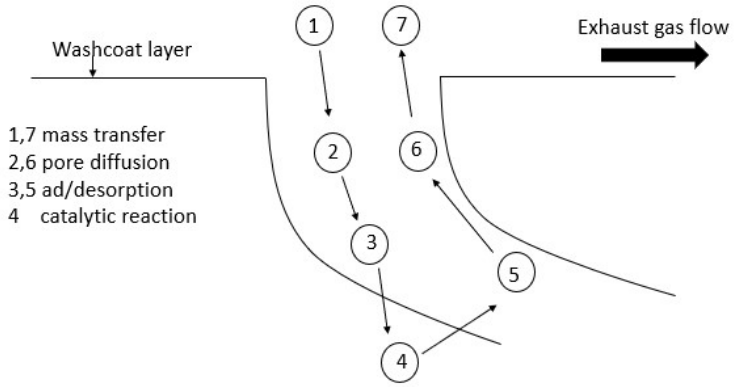


Figure 2.2: catalytic reduction

The chemical equation for the stoichiometric reaction with aquies ammonia is from the equation 2.1, 2.2 and 2.3 respectively.

$$2NO + 2NH_3 + \frac{1}{2}O_2 \rightarrow 2N_2 + 3H_2O \tag{2.1}$$

$$NO_2 + 2NH_3 + \frac{1}{2}O_2 \rightarrow \frac{3}{2}N_2 + 3H_2O \tag{2.2}$$

$$NO + NO_2 + 2NH_3 + \frac{1}{2}O_2 \rightarrow 2N_2 + 3H_2O \tag{2.3}$$

2.3 Chemical Reaction Rate Equations

Theoretically, we know that in the catalyst number of reactions happens, in this project kinetic modeling reaction rate calibration is carried for the most important chemical kinetics. For a chemical rate expression, representation of the general Arrhenius equation is shown in below equation 2.5.

$$Rate = k[X]^a[Y]^b \tag{2.4}$$

$$k = A * exp\left(\frac{-E_a}{RT}\right) * (conc) * (cov) * K(i) \tag{2.5}$$

where, A $\rightarrow$ pre-exponent multiplier,
E_a $\rightarrow$ activation energy or temperature,
R $\rightarrow$universal gas constant, 8.314j/mol K,
(conc) $\rightarrow$ concentration expressions,
(cov) $\rightarrow$ coverage expression,
K(i) $\rightarrow$ inhibition function,

All the reactions occur instantly at the same time, for simplifications of the modeling prediction the sequence of calibration methodology is described in chapter 3. The chemical reaction equation 2.6 and equation 2.7 are ammonia storage and desorption on the site elements respectively. The oxidation equation 2.8 some amount of ammonia is consumed or burned at higher temperatures. Then the most important $DeNO_x$ standard reaction, equation 2.9, consists of 90% of NO_x through denitrification the toxic elements are converted to simple components water and nitrogen. Followed by, $DeNO_x$ fast and $DeNO_x$ slow reaction which consists of only 10% of NO_x and occurs rarely.

R1 $$NH_3 + S \rightarrow NH_3(S) \tag{2.6}$$

R2 $$NH_3(S) \rightarrow NH_3 + S \tag{2.7}$$

R3 $$4NH_3(S) + 3O_2 \rightarrow 2N_2 + 6H_2O \tag{2.8}$$

R4 $$4NH_3(S) + 4NO + O_2 \rightarrow 4N_2 + 6H_2O \tag{2.9}$$

R5 $$2NH_3(S) + NO + NO_2 \rightarrow 2N_2 + 3H_2O \tag{2.10}$$

R6 $$8NH_3(S) + 6NO_2 \rightarrow 7N_2 + 12H_2O \tag{2.11}$$

The respective reaction rate expressions are shown below from equation 2.12 to 2.17 and it has several unknown terms to calibrate which defines the species outlet mole fraction curve.

$$\dot{r_1} = K_1.C^L_{NH_3}.(Z_{NH_3,max} - Z_{NH_3})^m \tag{2.12}$$

$$\dot{r_2} = K_2.Z_{NH_3} \tag{2.13}$$

$$\dot{r_3} = K_3.Z_{NH_3} \tag{2.14}$$

$$\dot{r_4} = K_4.C^L_{NO}.Z^*_{NH_3}.\left[1 - exp\left\{\left(\frac{-Z_{NH_3}}{Z^*_{NH_3}}\right)\right\}\right] \tag{2.15}$$

$$\dot{r_5} = K_5.C^L_{NO}.C^L_{NO_2}.Z^*_{NH_3}.\left[1 - exp\left\{\left(\frac{-Z_{NH_3}}{Z^*_{NH_3}}\right)\right\}\right] \tag{2.16}$$

$$\dot{r_6} = K_6.C^L_{NO_2}.Z^*_{NH_3}.\left[1 - exp\left\{\left(\frac{-Z_{NH_3}}{Z^*_{NH_3}}\right)\right\}\right] \tag{2.17}$$

where,

$$K_i = k^0_i.exp\left\{\left(\frac{-T_{A,i}}{T_{solid}}\right)\right\} \tag{2.18}$$

$$K_2 = k^0_2.exp\left\{\left(\frac{-T_{A,2}.(1- \in .Z_{NH_3})}{T_{solid}}\right)\right\} \tag{2.19}$$

m $\rightarrow$ adsorption order,
$\in \rightarrow$ epsilon,
S $\rightarrow$ site element,
$C_{NH_3} \rightarrow$ respective concentration species,
$Z_{NH_3,max} \rightarrow$ site coverage fraction,
$Z^*_{NH_3} \rightarrow$ critical fraction.
C^L_i is the concentration of species 'i' in the respective surface layer

2.4 Simplex and Genetic Algorithm

To perform the characterization process to optimize the unknown parameters initially manual calibration is performed to quickly bring the values to fall into the objective function direction. The integrated design optimization tool is utilized in GT-SUITE to find the closest possible magnitudes. The Simplex algorithm is a local optimizer that will converge to a local minimum used for the linear problems but here though it is non-linear, with numerous factors and multiple constraints it aids in finding design space with minimum efforts. In addition, there are many 3rd party tools for the optimization process for example, Matlab and Simulink which is not used because it stands out side the project scope.
The widely used for highly complex problems is Genetic Algorithm.[7]

- It can be applied for several unknown parameters for most complex problems.
- It is a 'sweep factor' that can find a single optimized value for all cases.
- If more number of generations, for example, 200 generations will trace very high log space math functions.
- Wide parameter range can be assigned, despite high computational time, can find the minimum objective function comparatively.

2.5 Calibration Requirements

The important requirements for the calibration process are the amount of exhaust gas flow composition with temperature programmed profile (TPD) and the chemical rate expressions. Once the inlet section is considered with the boundary condition profiles, parameter tuning to match with the experimental data by utilizing optimization tools within GT-SUITE. To optimize the objective function initially manual or trial and error method is carried generally to find the appropriate kinetic modelling to result in local minimum followed by the search algorithm to find the complex functions for multiple unknowns. The name of the reactions calibrated consisting of unknown parameters and the target terms are shown in **2.1** above. Furthermore, the calibrated catalyst continued with validation process for many experimental conditions for steady state and transient cycles. The calibration requirements flow chart is shown in **Figure 2.3**.

Table 2.1: Reactions with parameters and targets

	Reaction Name	**Unknown Parameter**	**Target**
R1	Adsorption	A, E, m, Site Density	ammonia adsorb
R2	Desorption	A, E, Epsilon	ammonia desorb
R3	Oxidation	A, E	ammonia with N_2 products
R4	$DeNO_x$ Standard	A, E, Critical Fraction	NO
R5	$DeNO_x$ Fast	A, E, Critical Fraction	NO and NO_2
R6	$DeNO_x$ Slow	A, E, Critical Fraction	NO_2

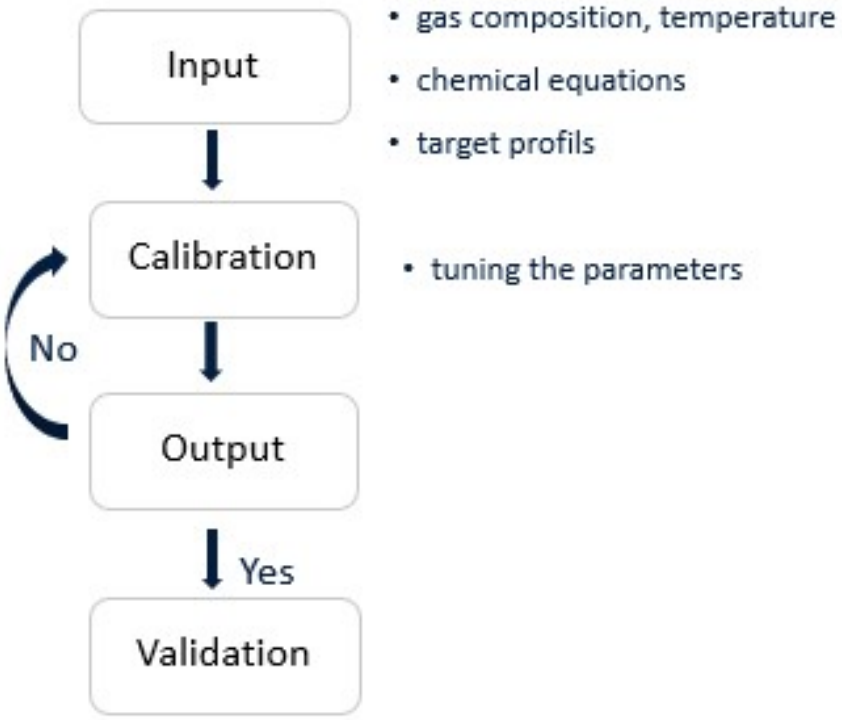


Figure 2.3: The requirements for the calibration process

3
Methodology

This chapter explains the project investigations in detail from building the SCR catalyst model in GT-SUITE v2020 to calibration steps involved and validation process. The flow chart below from the **Figure 3.1** represents the complete structure of the project. To begin with, the selective catalytic reaction (SCR) rate calibration is performed initially by applying physical properties of the catalyst for example diameter, length and area. Furthermore, either scat-rig data that is physically measured data or the digital laboratory Simulink black-box is utilized to generate target curve data for all the surface reaction mechanism method. Finally, the validation is performed using urea stairs and transient cycle experimental data against world harmonized transient driving cycles (WHTC) conditions.

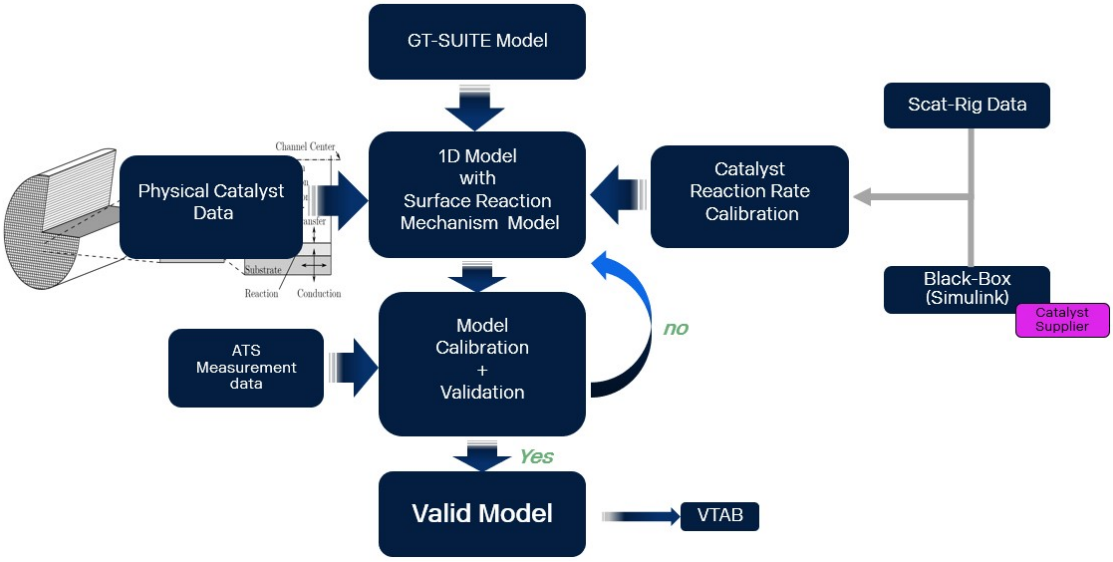


Figure 3.1: project structure

3.1 Building SCR Catalyst in GT-SUITE

The steps involved in building the SCR Catalyst model in GT-SUITE are explained in the chapter Appendix workflow documentation. Firstly, target data is produced from the Simulink black-box model. Calibration optimization is about minimizing the error or objective function between the target curves and GT simulation data. The most important reactions are from equation 2.6 to equation 2.11 used in reaction rate calibration, built-in SCR catalyst model in GT-SUITE v2020 is shown in

Figure 3.2 below.

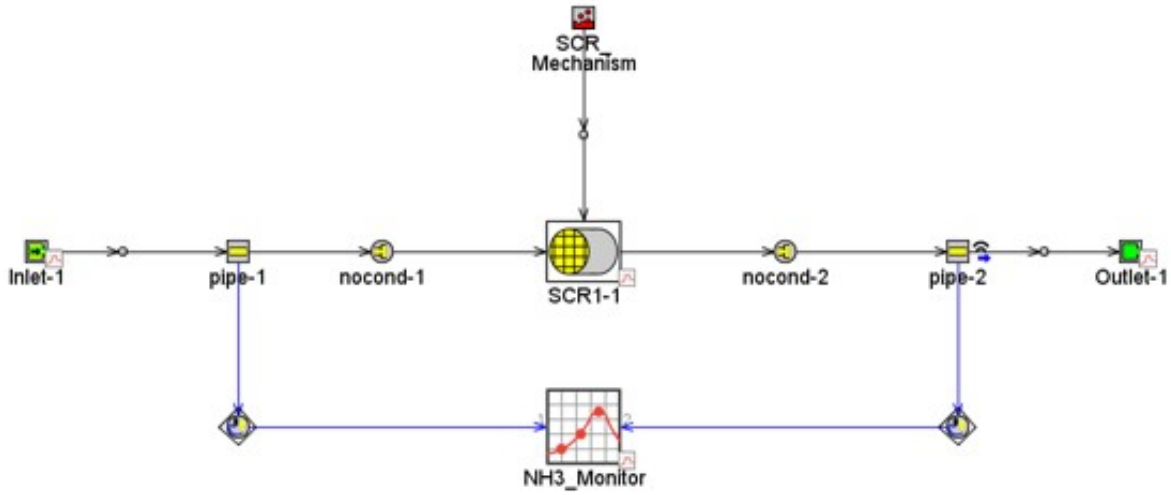


Figure 3.2: SCR Catalyst in GT-SUITE

The SCR Calibration Mechanism steps are explained briefly,

Step 1: The exhaust gas mass flow rate, inlet gas composition species from the engine out are introduced to the inlet section with temperature programmed desorption (TPD) profile.

Step 2: The physical and thermal properties are represented in SCR catalyst. For instance frontal area, length, cell density and wall temperatures and so on.

Step 3: In the SCR mechanism template all the reaction rate equations and the storage capacity of the catalyst are defined from general Arrhenius reaction rate equation as in equation 2.5.

Step 4: The components linked for chemical and physical flow characteristics and model is ready to run.

Step 5: Tuning or optimizing the unknown parameters to compare against target curve data sets.

3.2 Target Data from Simulink Black-box

In this project, a digital laboratory called simplified Simulink black-box model provided by the suppliers is utilized in producing the target data curves and is a necessary requirement for chemical kinetics modeling. From the boundary condition synthetic gas or constant gas are considered at the inlet section to measure the outlet data. The arrangement of the Simulink black-box model is in **Figure 3.3** and is mainly divided into three sections as inlet, catalyst and outlet section. The mass flow rate, temperature and species composition boundary conditions for the inlet. The physical property data and initial temperature are entered in the catalyst eventually outlets are measured and noted. The details of the target curve extraction method is explained for all the reactions from the below sub-section 3.3.1 to 3.3.5.

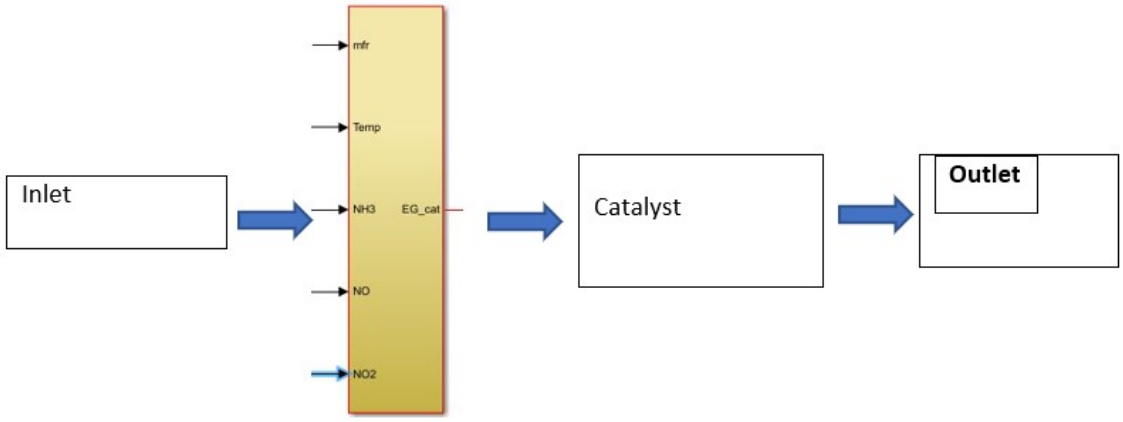


Figure 3.3: Simple representation of Simulink black-box model

3.2.1 Storage Target

For the storage calibration referred to the equation 2.6 and equation 2.7, constant temperatures 200°C, 300°C, 400°C and 500°C are considered, with the varied amount of ammonia concerning time as shown in **Table 3.1**. It is also important to respect the parameter limits provided by the suppliers hence the minimum amount of oxygen and water is taken into account. The outlet ammonia mole fraction data is collected for all the temperature conditions and the amount of oxygen and water shown below.

Table 3.1: Inlet ammonia composition for all temperature ranges

Time, sec	NH_3**, ppm**
0	0
100	0
100	1000
500	1000
500	500
700	500
700	250
1000	250
1000	0
1500	0
mass flow rate	0.002 kg/s
O_2	5000 ppm
H_2O	5000 ppm

3.2.2 Oxidation Target

The constant ammonia is fed at the inlet section with water and oxygen for several constant temperature conditions 250°C, 300°C, 350 °C, 400°C, 450°C, 500°C and 550°C. Ammonia outlet mole fraction data is measured and collected at the outlet. The amount of inlet species are shown below.

mass flow rate	0.002 kg/s
NH_3	1230 ppm
O_2	75000 ppm
H_2O	75000 ppm

3.2.3 DeNO$_x$ Standard Target

In the standard reaction rate equation referring to equation 2.15. NO concentration is the major species hence NO outlet mole fraction is collected. The experimental temperature ranges are same as that of the oxidation. The boundary condition inlet species are shown below.

mass flow rate	0.002 kg/s
NH_3	600 ppm
NO	500 ppm
O_2	85400 ppm
H_2O	50000 ppm

3.2.4 DeNO$_x$ Fast Target

In the DeNOx fast reaction equation, it contains of both NO and NO_2 concentrations hence the outlet mole fractions of both NO and NO_2 are measured. The boundary condition inlet species are shown below.

mass flow rate	0.002 kg/s
NH_3	600 ppm
NO	250 ppm
NO_2	250 ppm
O_2	85400 ppm
H_2O	50000 ppm

3.2.5 DeNO$_x$ Slow Target

During slow reaction rate calibration only NO_2 concentration species are captured and the inlet conditions are shown below.

mass flow rate	0.002 kg/s
NH_3	600ppm
NO	125ppm
NO_2	375ppm
O_2	85400ppm
H_2O	50000ppm

3.3 Calibration Process

The selective catalytic reduction (SCR) seems the most promising technology to eliminate toxic emissions nitrogen dioxide NO_x from diesel engines with the aid of reducing agent ammonia or urea or adblue. The reaction rate calibration is performed by modeling surface reaction kinetics for six rate expressions and 18 unknown parameters to calibrate as shown in **Table 2.1**. All the reaction rate calibration process are described from the below section 3.4.1 to section 3.4.6.

3.3.1 Thermal Calibration

The temperature of the catalyst is directly proportional to the chemical reactions because it influences the start of the reaction or activation rate of reaction. Hence, SCR catalyst model is tested to study the thermal behaviours to match with the output from the experiments, by feeding the same amount of temperature ramp

for both GT-Model and Simulink as shown below table. The intrinsic density of substrate cordierite material is tuned or adjusted to match with the output from Simulink experiments, blue line and compared with the GT-model, red line, in below **Figure 3.4**.

Time, sec	**Temperature,°C**
0	20
500	400

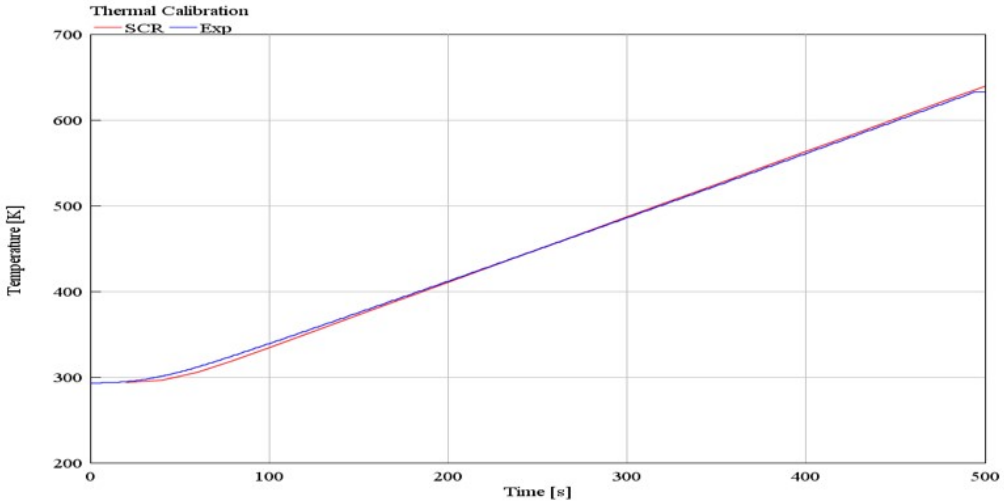


Figure 3.4: Thermal calibration

3.3.2 Storage Calibration (Adsorption Desorption)

The arrangement of SCR catalyst model along with surface reaction mechanism model is shown in the **Figure 3.5** below. For the chemical reaction to happen initially ammonia has to be stored on the surface of the catalyst. The chemical rate expression is shown in equations 2.10 and 2.11 respectively. There are seven parameters to calibrate during storage calibration they are,

active site density | A_1 | E_1 | A_2 | E_2 | m, adsorption order | $\in$,epsilon

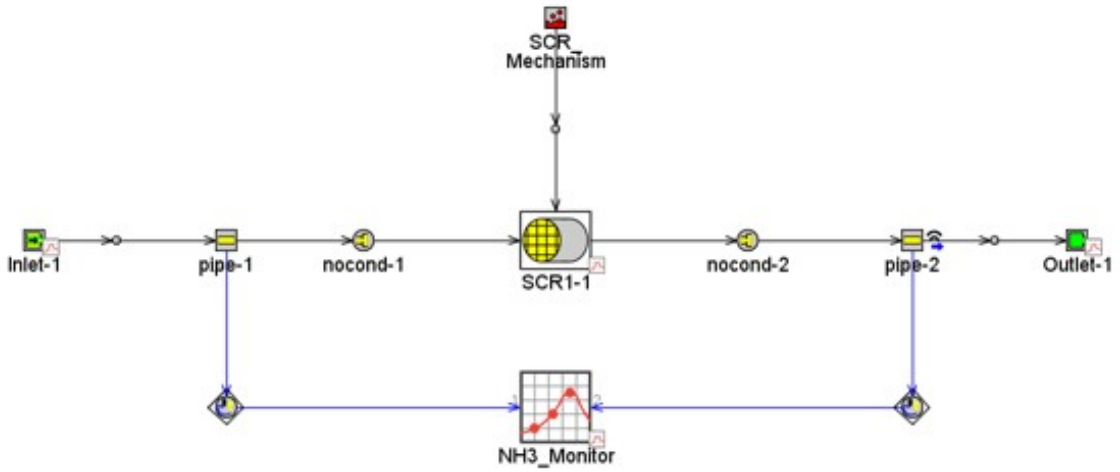


Figure 3.5: SCR Catalyst in GT-SUITE

The active site density in mole/cm^3 indicates the amount of ammonia it can store and so is a parameter. During storage of ammonia, it can also desorb mainly because when the site element is becoming full, if the temperature and pressure conditions are satisfied some amount of ammonia consumed. From the external pipe ammonia is sprayed to mix with exhaust gas flow and NH_3 settles on the porous site elements of the catalyst. The experiments are conducted for constant temperature ranges 200°C, 300°C, 400°C and 500°C respectively by activating respective rate equations. In the inlet section, the constant mass flow rate 0.002 kg/s, constant temperature 200°C and gas composition from **Table 3.3** is the boundary condition. The outlet ammonia mole fraction captured is referred from the **Figure 3.6**, initially ammonia is adsorbed up to 220sec so the curve is steep and reaches a constant of about 1000ppm and ammonia is stored untill 500sec then desorption starts from 500sec to reach zero gradually. The green line is the inlet ammonia profile, the experimental outlet species data, red line, overlaps closely with the GT simulation outlet species, blue line.

Initially, the model run with approximate parameter values with respect to target profile data, simulation dashboard successfully generates the GT-Power file eventually necessary results are compared. After several manual trials, integrated design optimizer; simplex and genetic search algorithm is utilized to optimize the unknown parameters in quick time, up-to 500 runs iteration to find the closest possible parameter values to match with the experimental data. In other words, these parameter values defines the outlet mole fraction curve.

Table 3.2: Inlet composition in mole fraction for storage calibration

Time, sec	N_2	O_2	CO	NH_3	NO	NO_2	H_2O	N_2O
0	0.9	0.05	0	0	0	0	0.05	0
100	0.9	0.05	0	0	0	0	0.05	0
100	0.899	0.05	0	0.001	0	0	0.05	0
500	0.899	0.05	0	0.001	0	0	0.05	0
500	0.8995	0.05	0	0.0005	0	0	0.05	0
700	0.8995	0.05	0	0.0005	0	0	0.05	0
700	0.89975	0.05	0	0.00025	0	0	0.05	0
1000	0.89975	0.05	0	0.00025	0	0	0.05	0
1000	0.9	0.05	0	0	0	0	0.05	0
1500	0.9	0.05	0	0	0	0	0.05	0

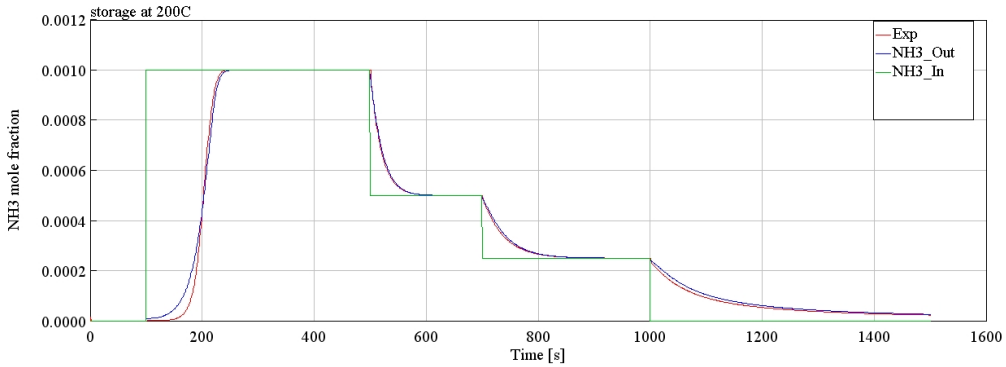


Figure 3.6: Ammonia Storage at 200°C

All the set up remains same and observed that target curve data closely match with the GT-model output for 300°C and is shown in **Figure 3.7**.

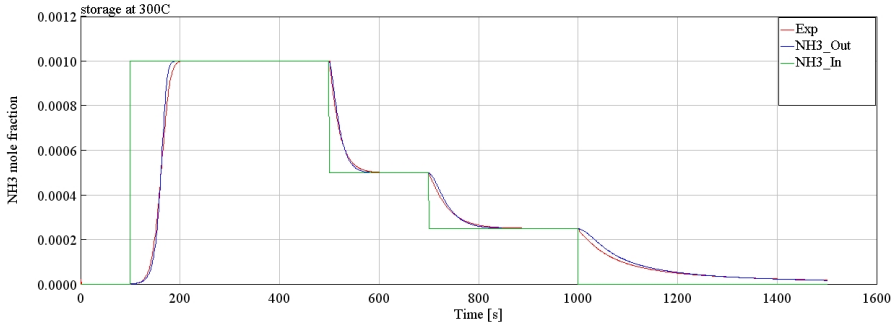


Figure 3.7: Ammonia Storage at 300°C

At high constant temperature experimental condition 400°C and 500°C in below **Figure 3.8** and **Figure 3.9** represents the outlet ammonia species experimental profiles respectively. The ammonia is consumed at very high temperatures after 350°C because of oxidation effect.

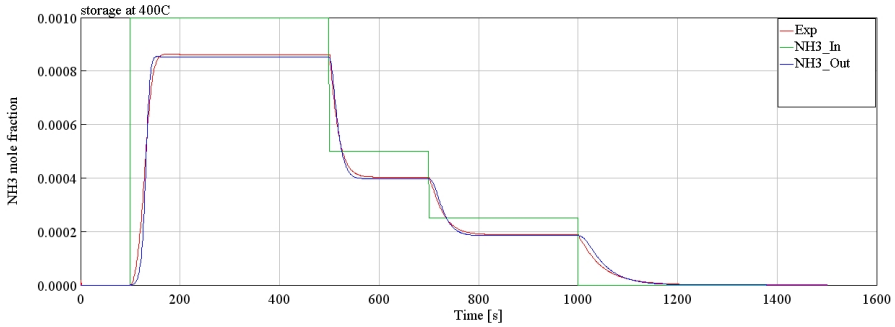


Figure 3.8: Ammonia Storage at 400°C

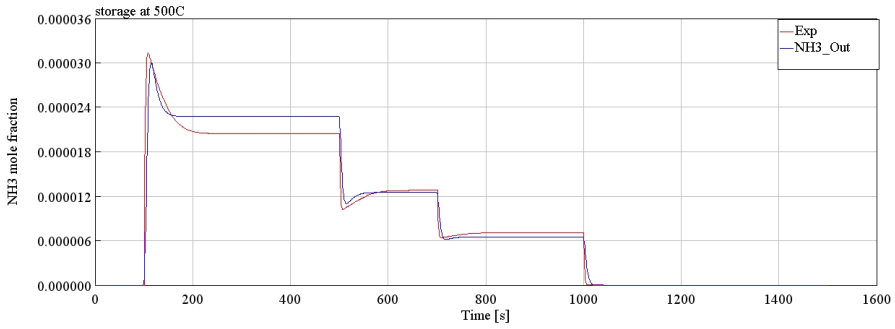


Figure 3.9: Ammonia Storage at 500°C

3.3.3 Oxidation Reaction Rate Calibration

The arrangement of the SCR catalyst in the GT model remains unchanged but the experimental inlet conditions vary. In the oxidation reaction rate calibration experiment, constant inlet conditions are referred to the **Table 3.4**. The seven parameters values obtained in the previous step are fixed, so A_3 pre-exponent multiplier and E_3 activation energy are two parameters from equation 2.12. The adsorption, desorption and oxidation rate expressions are active in the surface mechanism templet. The optimal temperature condition ranges from 250°C to 550°C are performed,**Figure 3.10** is the comparison of ammonia outlet mole fraction against temperatures, where NH_3 inlet, green line, NH_3 outlet from experiments, black line, and GT model simulations, orange line. The oxidation is highly active at higher temperatures after 350°C.

Table 3.3: Inlet composition during oxidation reaction rate calibration

Time, sec	N_2	O_2	CO	NH_3	NO	NO_2	H_2O	N_2O
0	0.873	0.075	0	0.00123	0	0	0.05	0
500	0.873	0.075	0	0.00123	0	0	0.05	0

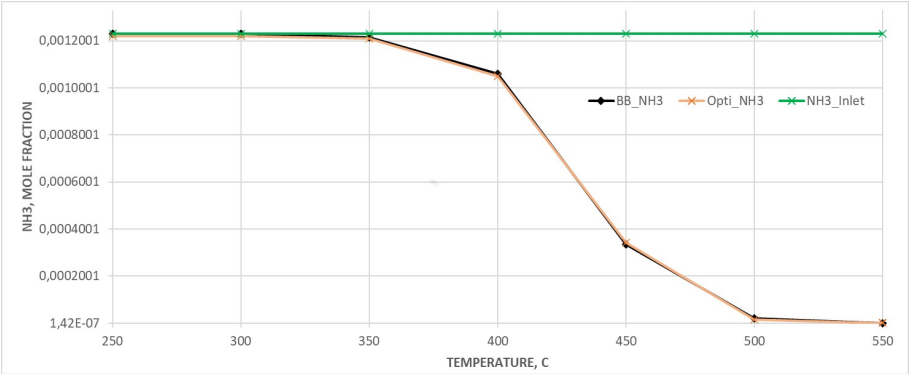


Figure 3.10: Oxidation outlet molefraction comparision

3.3.4 DeNO$_x$ Standard Reaction Rate Calibration

The standard rate expression from equation 2.13 consists of concentration of nitrogen oxide NO hence during standard reaction rate calibration toxic substance NO_x are dismantled into harmless simple component significantly. The experimental temperature remains same as that of oxidation and inlet composition are in **Table 3.5** below.

Table 3.4: Inlet composition during standard reaction rate calibration

Time, sec	N_2	O_2	CO	NH_3	NO	NO_2	H_2O	N_2O
0	0.8635	0.0854	0	0.0006	0.0005	0	0.05	0
500	0.8635	0.0854	0	0.0006	0.0005	0	0.05	0

There are three parameters to calibrate, A_4, E_4 and B - critical fraction. The **Figure 3.11** is the outlet conversion rate for the NO mole fraction comparison between experimental or Simulink black-box data, black line and GT-simulations data orange line. Noticeably, at low temperature 250°C outlet mole fraction is slightly higher in simulations and is almost negligible.

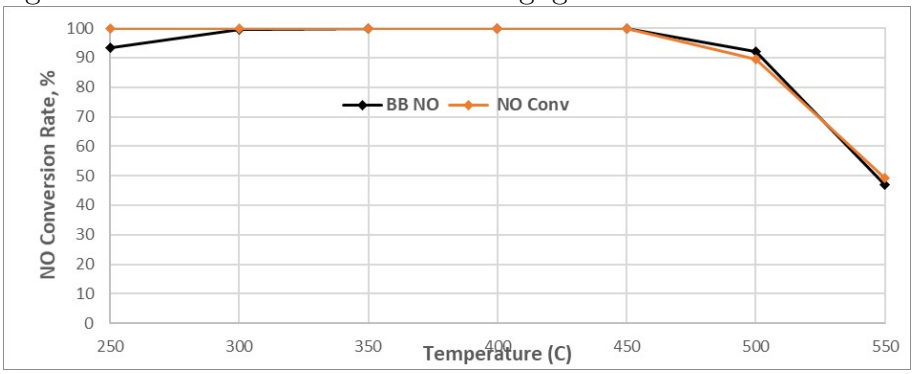


Figure 3.11: DeNO$_x$standard outlet NO conversion rate comparison

3.3.5 DeNO$_x$ Fast Reaction Rate Calibration

The fast expression rate equation 2.14 consists of NO and NO_2 concentrations so outlet mole fractions of both NO and NO_2 are captured and the conversion rates comparison are shown in **Figure 3.12** and **Figure 3.13** respectively. A_5, E_5 and B - critical fraction are the unknown parameters. At very high temperature after 450°C simulation outlet mole fraction, orange line is quite off for NO, from experiments

data we know that the operating boundary condition temperatures are below 400°C and is focused on low temperatures to move with validation. The inlet composition conditions are shown in **Table 3.6**.

Table 3.5: Inlet composition during fast reaction rate calibration

Time, sec	N_2	O_2	CO	NH_3	NO	NO_2	H_2O	N_2O
0	0.8636	0.0854	0	0.0006	0	0.000375	0	0.05
500	0.8636	0.0854	0	0.0006	0	0.000375	0	0.05

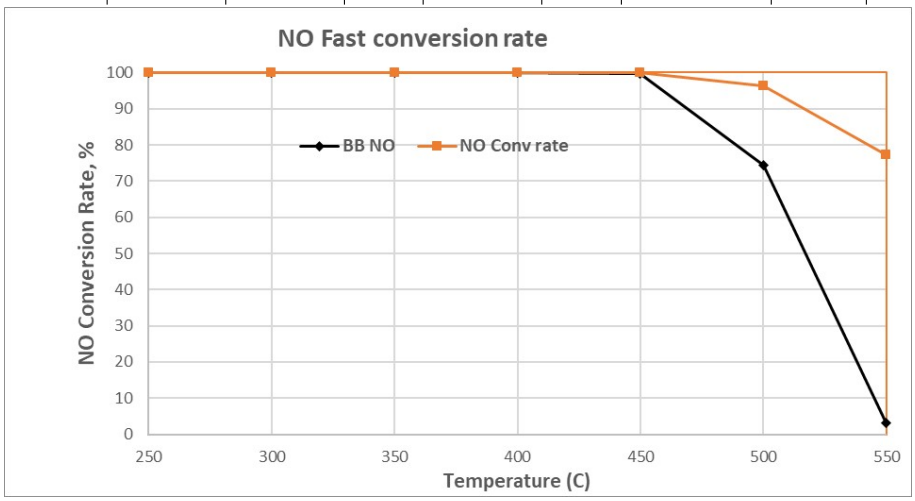


Figure 3.12: DeNO$_x$ fast outlet NO conversion rate comparision

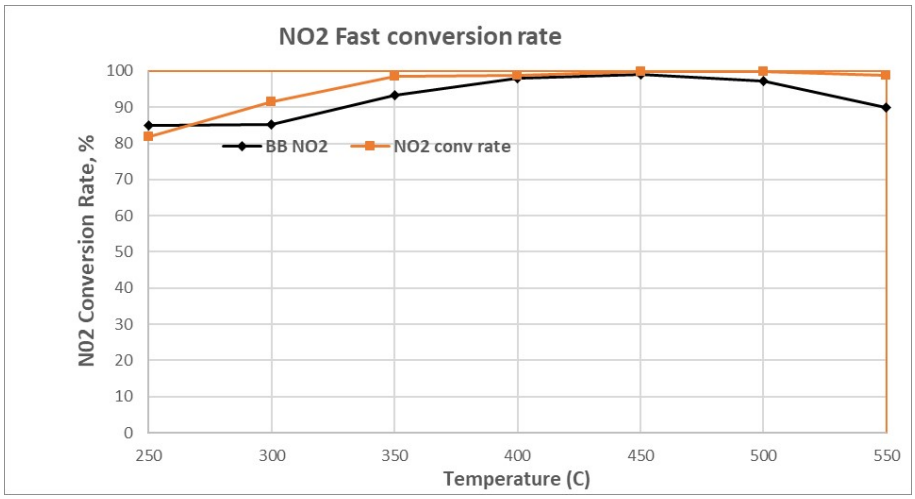


Figure 3.13: DeNOx fast outlet NO_2 conversion rate comparision

3.3.6 DeNO$_x$ Slow Reaction Rate Calibration

From equation 2.15, NO_2 is the major composition species. However, NO_2 outlet mole fraction conversion is shown in **Figure 3.14** and the simulated curve almost fits with the experiments.

Table 3.6: Inlet composition during slow reaction rate calibration

Time, sec	N_2	O_2	CO	NH_3	NO	NO_2	H_2O	N_2O
0	0.8636	0.0854	0	0.0006	0	0.000375	0	0.05
500	0.8636	0.0854	0	0.0006	0	0.000375	0	0.05

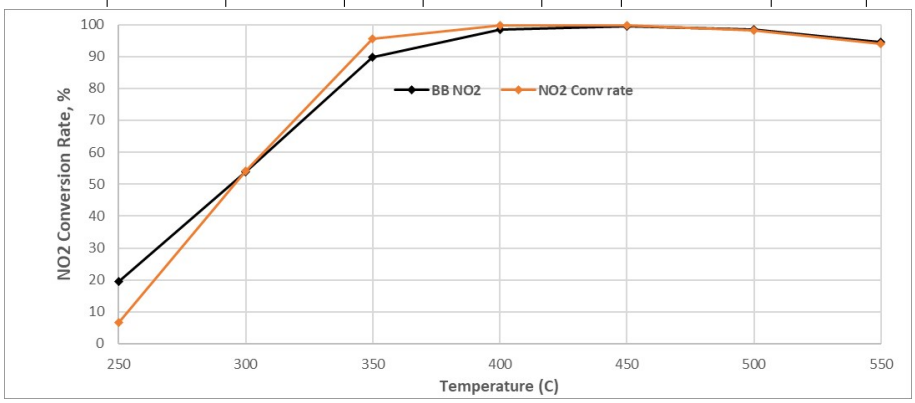


Figure 3.14: DeNOx slow outlet NO_2 conversion rate comparision

4

Validation

This chapter describes the validation method basically to accomplish the requirements of typical driving conditions for heavy-duty Euro V legislative regulation certifications. The calibrated chemical kinetics model connected to the SCR catalyst to perform several experiments for urea stairs, US, cases and transient driving cycle analysis. In the validation model engine-out exhaust gas composition, temperature profile and mass flow rate boundary conditions are introduced at the inlet, followed by adblue dosing unit and two split SCR connected with calibrated chemical kinetics model to measure the amount of NO_x reduced at the outlet. Moreover, the monitor reads all the signals from inlet to outlet. **Figure 4.1** shows the arrangement of the exhaust aftertreatment validation model in GT-SUITE. Here, adblue solution is injected through a global templet external source connected just before SCR, where there is no desire to capture thermolysis and hydrolysis kinetics.

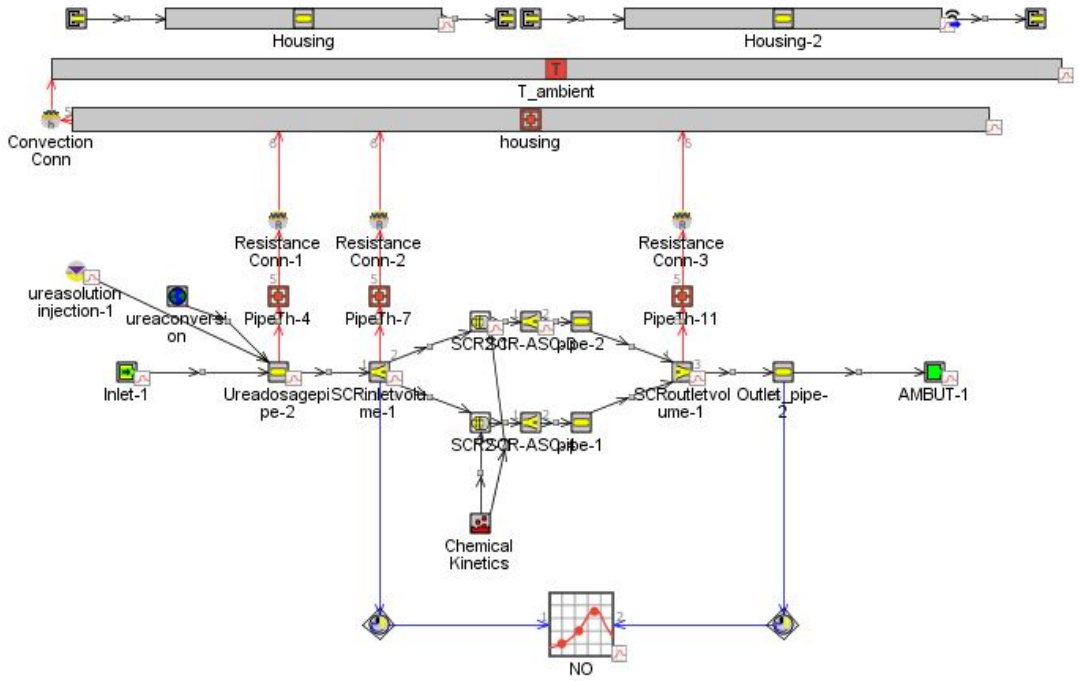


Figure 4.1: GT-SUITE validation model

The approach to achieve 100% adblue decomposition by setting up the activation energy to zero and pre-exponent multiplier is adjusted to large enough number to ensure all conversion at all times from adblue to urea to NH_3 in the global reaction templet. The global reaction is shown in equation 4.1 below.

$$UreaSolution, 0.2524NH_3 + 0.1262CO_2 \rightarrow 2N_2 + 0.7476H_2O(vapor) \quad (4.1)$$

4.1 Steady State or Urea Stairs Validation

The several experiments for different mass flow rates and temperature urea stairs, US, conditions performed for the analysis of the Euro V validation and description are explained below.

4.1.1 Steady State Experiment 1: Low Mass Flow Rate

The engine-out exhaust gas composition, temperature profiles and mass flow rate are the inlet boundary condition data. Followed by adblue dosing through global template injection pipe, chemical kinetics are attached to the SCR to study the amount of NO_x reduced at the outlet. Evidently, with the increase in dosage of adblue injection high chance to reduce NO_x significantly. The outlet ammonia slip and outlet NO_x reduction conversion rate in percentage for different steps were compared in **Figure 4.2** below. The X-axis is the experimental steps and the y-axis, left, is outlet NO_x in % and y-axis, right, NH_3 slip in %. During low mass flow rate 540C kg/h the ammonia slip in the GT model is well captured except at step eight. Also, the NO_x in the GT-model overlaps with the experimental outlet NO_x, but minor error at step two, assuming because of inlet composition error or an unknown error in the model but later it overlaps with the experiments. The dash black line are experiments NH_3 and NO_x, light green is NH_3 slip and brick red is NO_x GT respectively referring to the **Figure 4.2**.

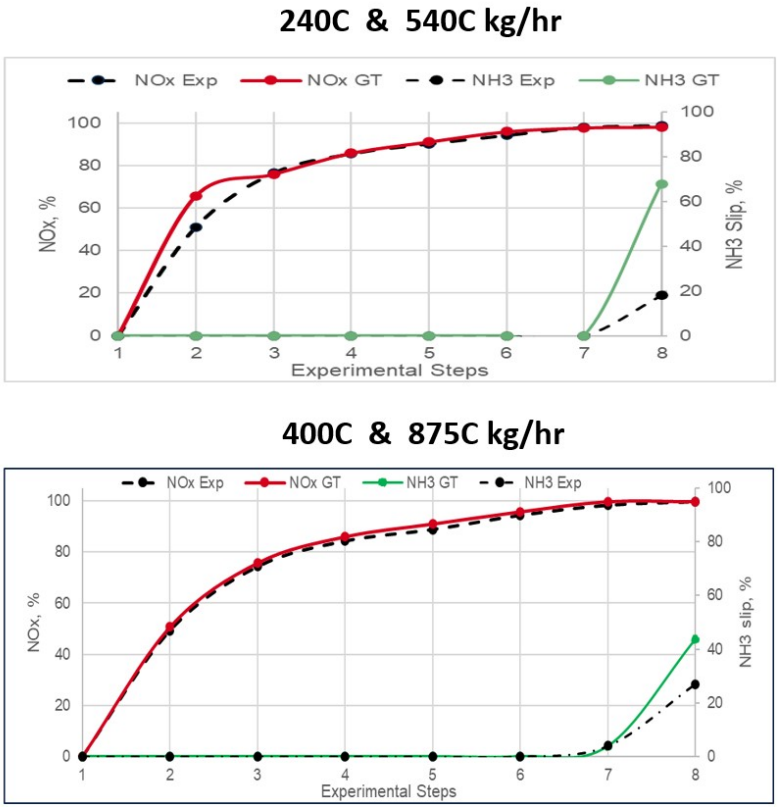


Figure 4.2: Low mass flow rate comparison

4.1.2 Steady State Experiment 2: Medium Mass Flow Rate

In the experiment 2, NH_3 slip is early from step two but with high discrepancy compared to the previous experiment case this is mainly because of high mass flow rates 1350kg/h and 1660kg/h. The outlet NO_x is well captured in GT model for 1350kg/h but the NO_x over predicts for 1660kg/h and shown in the **Figure 4.3**.

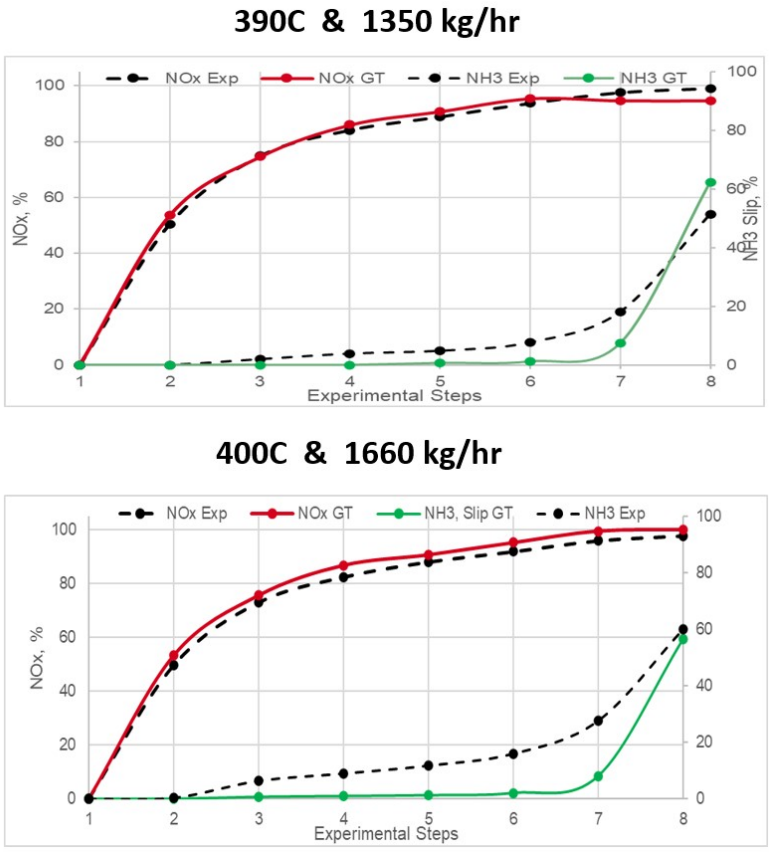


Figure 4.3: Medium range mass flow rate comparison

4.1.3 Steady State Experiment 3: High Mass Flow Rate

In the experiment 3, further increase in mass flow rate discrepancy also increases comparatively to low and high mass flow rate experiments. From **Figure 4.4** the NO_x in GT-model simulations from step three is quite off and also ammonia slip is high in experiments. The factors aiding discrepancy at higher mass flow rate are explained in the section 4.3.

Overall, for the steady state experimental results, there is no temperature effect for NO_x and NH_3 slip capturing but high mass flow rate affecting majorly to influence the discrepancy between simulated data and experimental data. There might be several reasons causing this discrepancy at higher mass flow rates and is clearly explained in section 4.3 and section 4.3.1

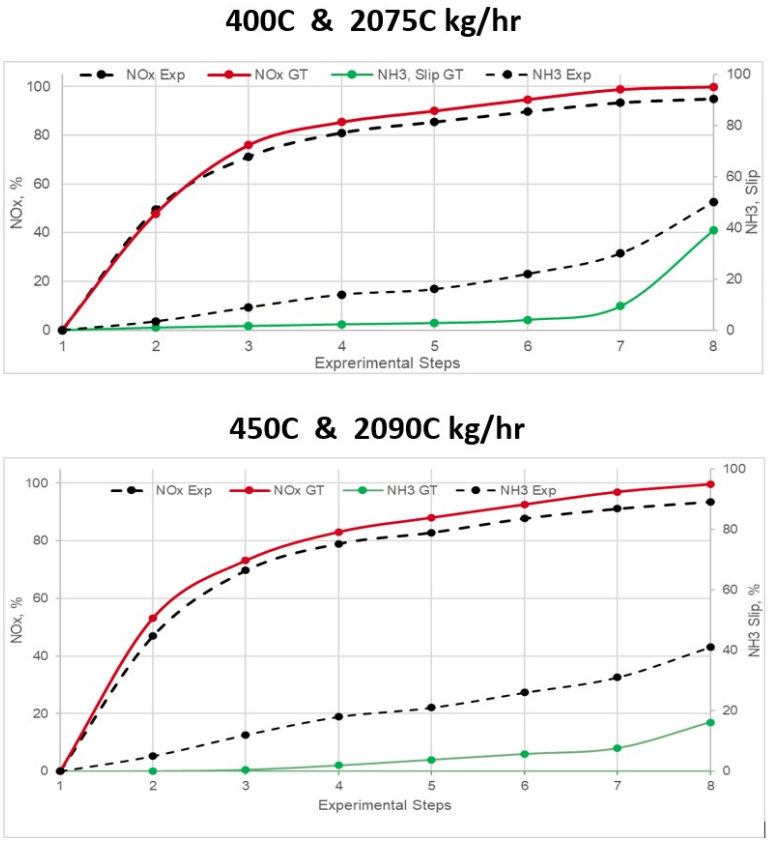


Figure 4.4: High range mass flow rate comparison

4.2 Transient State Validation

The validation is performed for several WHTC transient cycles for different ammonia NO_x ratio (ANR), conditions.

4.2.1 Ammonia NO_x ratio, ANR, 0.8

The experimental set up for varying temperature profile, exhaust mass flow rate and inlet gas composition is boundary condition at the inlet section. Followed by the adblue injection profile in the global reaction templet and mass flow rate are displayed in **Figure 4.5**. The blue colour is for NO_x and NH_3 from GT simulations where as orange line is from experiments. The outlet NO_x from GT is quite high compared to experiments but the NH_3 slip follows the same as that of experiments.

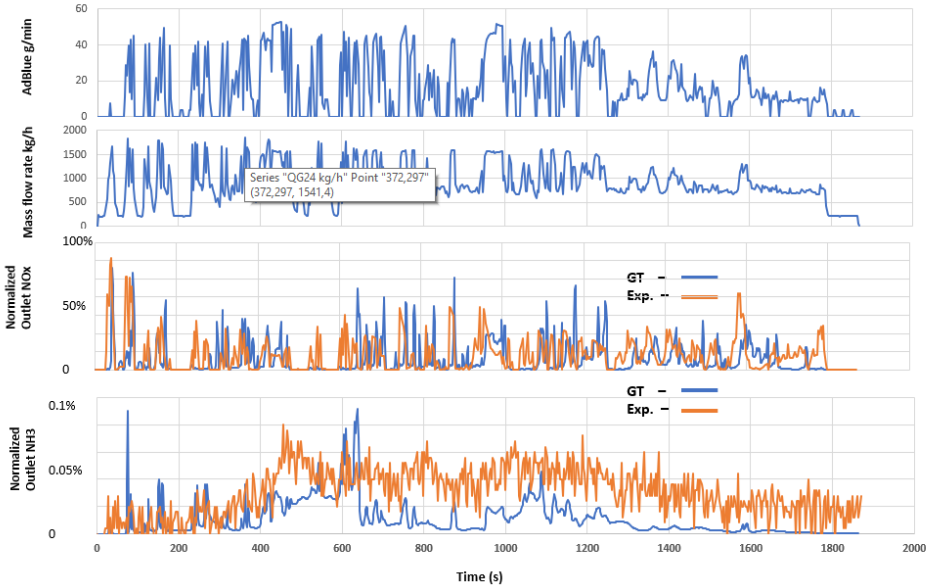


Figure 4.5: Ammonia NO_x ratio 0.8

4.2.2 Ammonia NO_x ratio, ANR, 0.9

The increase in adblue injection has an effect of more NH_3 slip in GT-model but the NO_x has significantly reduced. The NO_x and NH_3 slip trend is shown in the **Figure 4.6**. There is almost zero NO_x in GT around 500sec, the reasons causing this discrepancy are explained later in the section 4.3 and section 4.3.1.

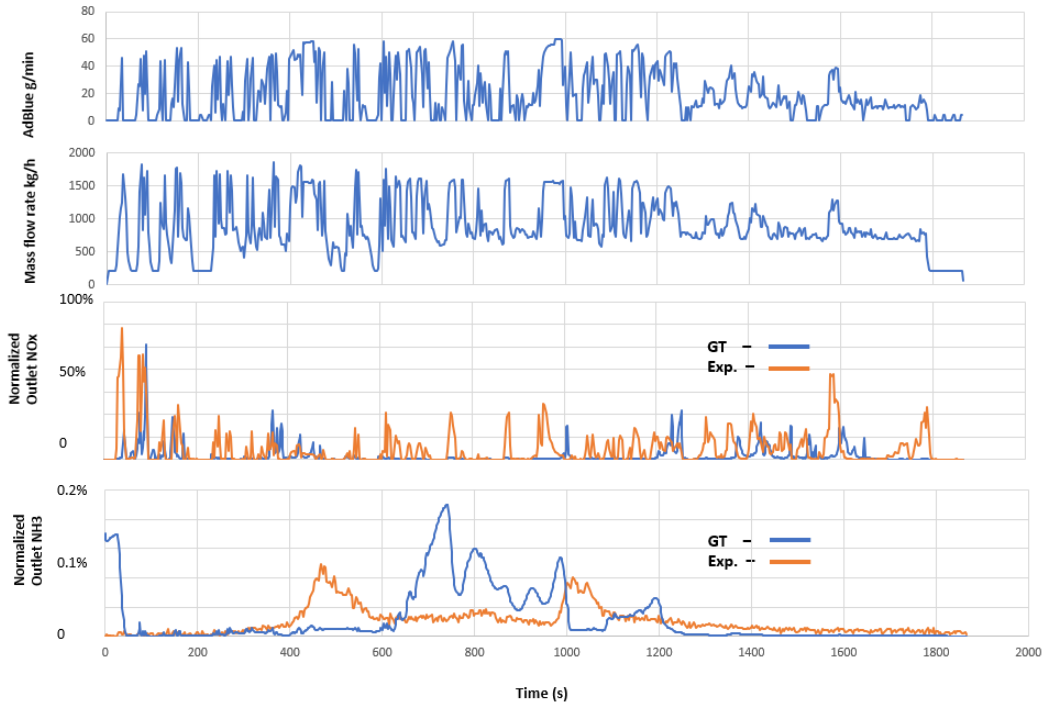


Figure 4.6: Ammonia NO_x ratio 0.9

4.2.3 Ammonia NO_x ratio, ANR, 1.1

Further increase in the adblue injection the outlet NO_x almost reduced to zero and outlet ammonia slip also follows the same trend as that of the experiments. The **Figure 4.7** compares the results for this experimental condition.

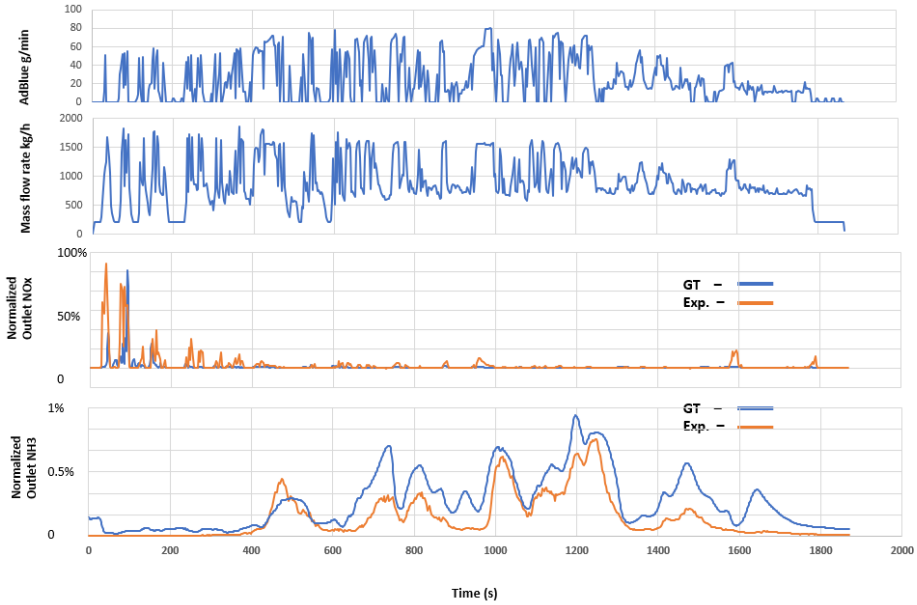


Figure 4.7: Ammonia NO_x ratio 1.1

4.3 Source of error at high mass flow rates

The considerable reasons impact the difference between the simulation results and the experiment results, the most important are highlighted here.

- **Temperature:** of course, temperature plays an influential role for the chemical reaction rate and as it is 1D modeling it is captured well in GT model. Overall, for all steady state experiments, the temperature doesn't influence much even for higher mass flow rate conditions. Refer to the **Figure** 4.3
- **Frontal area of the catalyst**: At higher mass flow rates because of high speed gas flow, the ammonia particles does not travel to the corner pores sites so high chance of improper utilization of the open frontal area of the catalyst. Hence, insufficient amount of ammonia to react with NO_x.
- **Ammonia NO_x Ratio (ANR):** It is defined as the ratio of one mole of ammonia reacts with one mole of NO_x during the chemical reaction for perfect mixing efficiency. At a low ANR scenario, insufficient amount of ammonia to react with NO_x hence one can expect low conversion efficiency, this causes discrepancy in experimental data compared to GT-model results.
- **Distribution Problems:** In reality, it is challenging to split the exhaust gas flow equally between the two SCR, this causes uneven flow of exhaust gas, uneven mixing so unreacted excess NH_3 left out at the outlet. This can be

addressed in the future projects, by implementing mixing and distribution models by extracting information from 3D CFD to 1D to achieve better model results.

4.3.1 Other factors for discrepancy between experiments and simulation results

The other non-negligible factors aiding discrepancy might also include as followed,

- Further improve in accuracy of reaction rate calibration especially at low temperature, will push the GT-model results much closer towards accuracy.
- The chemical reactions might occur in different forms, by introducing more chemical rate calibration reactions can predict better at the outlet NO_x in the catalytic reaction.
- The pressure and temperature drop calibrations in each components of the aftertreatment components, can surely effect the outcome of results because temperature is a dependent variable for the reaction rate. Also , during 1D modeling, it is important to care temperature and pressure drop between the components during gas flow.
- During physical measurements, it is difficult for the sensor's to capture the peak signals, especially for WHTC transient cycles because of high oscillation frequencies.
- Normally, measurement sensor devices are placed on the surface of the tail or engine out pipes which creates imprecise estimates in the pipe center.
- The utilization of different chemical solvers can improve the overall results.
- Gen 3 v/s Gen 4 catalyst: In this project, the tailpipe and engine out experiments were conducted for generation 4 catalyst, where as Simulink produces the experiments for generation 3. Though it is almost the same catalyst but the different one.
- Improved inlet conditions data: For the accuracy of the model results, it is also most important to collect the data requirements for the simulations, for instance, inlet gas composition and initial loading of NH_3 in the catalyst during several transient trials.
- The approach to convert urea solution to ammonia by capturing thermolysis and hydrolysis kinetics method can well define the amount of NH_3 needed to react with a toxic component in the catalyst. Implementing this models in GT will definitely improve the results in future to strengthen the arguments.

5
Conclusion

- This project is a strong foundation for the exhaust aftertreatment system development projects for the future.
- Overall, for the SCR calibrated catalyst we have reasonable results for the steady state or urea ”trappa” conditions but results can be further improved for transient state conditions by implementing mixing and distribution models in the future.
- The work flow was quite smooth through out the project, but there was delay in receiving the black box model at the beginning of the project and later in the second half we are able to expand the contacts with GT-support team, suppliers and other adjacent groups with in Scania. Hopefully, this will help for the projects in the future.

6
Future Work

In the future it would be interesting to improve the WHTC transient cycles results for the calibrated SCR catalyst by implementing the information from 3D to 1D this will include mixing and distribution modeling.

The calibration will be continued for other ammonia slip catalyst (ASC) and diesel particulate filter (DPF) to study the Euro 6 steady-state and transient state cycle validation.

The approach of handling urea solution can be better implemented by capturing thermolysis and hydrolysis kinetics. Hence conversion of urea to ammonia will be better handled to ensure no excess ammonia slip at the outlet and improves overall results of the validation process.

Bibliography

[1] Transport Resources International Ltd. European industry has se led on euro vi, May 2020. URL /www.dougjack.co.uk/bus-industry-euro-6-emissions-limits.html.

[2] Sangchul Ko 1,2, Junhong Park 1,*, Hyungjun Kim 1 , Gunwoo Kang 1 , Jongchul Lee 1 , Jongmin Kim 1 and Jongtae Lee 1 . Nox emissions from euro 5 and euro 6 heavy-duty diesel vehicles under real driving conditions, 2 January 2020.

[3] Euro 1 to 6 legislative regulations for heavy duty vehicles, 1996. URL https://dieselnet.com/standards/eu/hd.php.

[4] Felipe Rodríguez Pierre-Louis Ragon. Estimated cost of diesel emissions control technology to meet future euro vii standards, April 2021. URL EstimatedcostofdieselemissionscontroltechnologyforfutureEuroVIIstandards.

[5] Hiroki Ueno Kiminobu Hirata, Nobuhiko Masaki and Ltd. Hisashi Akagawa Nissan Diesel Motor Co. Development of urea-scr system for heavy-duty commercial vehicles, 2005-01-1860. URL https://www.sae.org/publications/technical-papers/content/2005-01-1860/.

[6] Xiaocheng Ma2 Jiantao Liu3 Xianping Zeng4 Jianxing Ren5 e Kunkun You1, a. Characteristic analysis of scr flue gas denitrification catalyst in power plant, 2012-05-14. URL https://www.scientific.net/AMR.518-523.2423.

[7] 2019 Gamma Technologies LLC. Gt suite optimization manual, Published : June 2019.

7
Appendix

GT-SUITE
GT-ISE

SCR Calibration Workflow Documentation
IN GT-SUITE

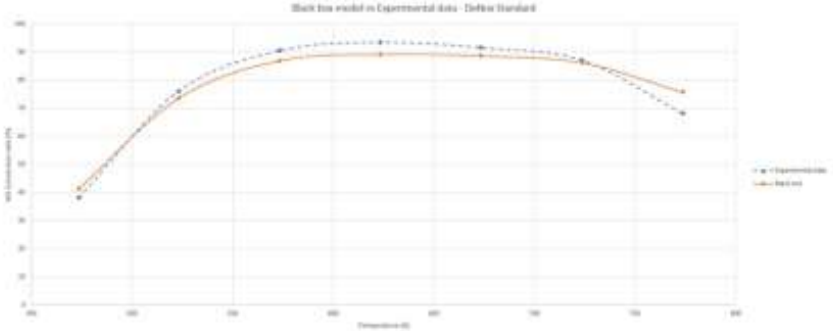
Spring 2021 (Feb - Sep)

Emissions Solution Development Department - NXPS

SCANIA

GT-SUITE
GT-ISE

Simulink black-box vs Experimental data



❖ Verification and comparision of the black-box outlet species data with measurement or experimental data to check the behaviour of the black-box model.

GT-SUITE simulation modelling and calibration

Measurement Data from Simulink Black-box
- Constant temperature
- Temperature programmed desorption (TPD)
- Species composition

GT-SUITE Modelling
- Inlet species composition with temperature profile
- SCR physical & thermal properties data
- Surface reaction mechanisem

Calibration Methodology
- Manual
- Design Optimizer (Genetic Algorithm)

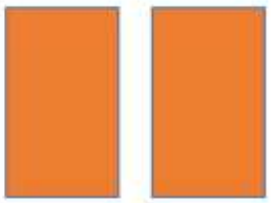
Method



- gas composition, temperature
- chemical equations
- Target profile or Experimental data

- Tuning the parameters

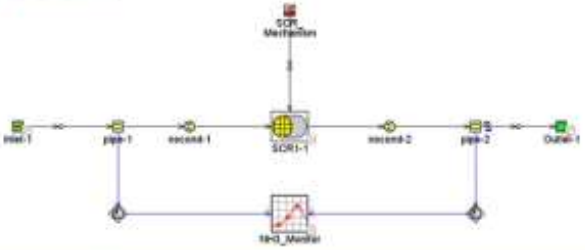
Catalyst Specifications



Substrate – Cordierite

Site Element – Vanadium

Building SCR Model in GT-SUITE



- ✓ The model is built with reference to the GT-tutorial
- ✓ Adsorption, Desorption and Oxidation are calibrated at the same time
- ✓ Standard reaction rate equation is calibrated alone
- ✓ Fast and Slow equations are calibrated together.

Reactions	Parameters	Equations	Target
1) Adsorption	A, E, M, site density	$V+NH_3 \longrightarrow VNH_3$	NH3 storage
2) Desorption	A, E, Epsilon	$VNH_3 \longrightarrow V+NH_3$	NH3 desorbtion
3) Oxidation	A, E	$4VNH_3+3O_2 \longrightarrow 2N_2+6H_2O+4V$	NH3 target, Oxidation with N2 product
4) DeNox Standard	A, E, B	$4VNH_3+4NO+O_2 \longrightarrow 4N_2+6H_2O+4V$	NO
5) DeNox Fast	A, E, B	$4VNH_3+2NO+2NO_2 \longrightarrow 4N_2+6H_2O+4V$	NO & NO2
6) DeNox Slow	A, E, B	$8VNH_3+6NO_2 \longrightarrow 7N_2+12H_2O+8V$	NO2

A - Pre-exponent multiplier

E - Activation temperature or energy in K

M – Adsorption order

B - Critical fraction

Steps involved in building an SCR model

Building the flow components

Open GT-SUITE and create a new GT-project map, go to File > Resources > Create New Model (Ctrl +N). In the model file, select GT-Model and choose either GT-Suite or GT-Power license. In the applications select exhaust after-treatment system for the preloading templets then finish.



1.1 Inlet Section

- The very first step is to create a new 'EndFlowInletSpecies' templet by double-clicking in the project library. Name as 'Inlet' enter mass flow rate , temperature and composition. To create a temperature profile right click and choose value selector or press the value selector button (box with three dots...) and then create new ProfileTransient object named temperature or open the square bracket and put the constant temperature for instance 100, 200, 300 and so on in the case setup.



- To the attribute composition time series from the value selector create a new XYTableMulti and name it as Comp_TPD. In the first row of the XYTableMulti array, click on the three dots(...) to go to the GT-library and choose n2-NASA hit ok and so on.



1.2 Pipe between inlet, outlet and catalyst



- The cone is identical, from the project library double-click on 'FlowSplitGeneral' and name it as 'Cone' for the initia state name, use valve selector to create new FluidinitialState refrence object named initial enter pressure and temperature for initial conditions.

1.3 SCR Catalyst Brick

- From the libraries click on 'CatalystBrick', punch in the physical and thermal properties of the catalyst. In the thermal tab, for substrate thermal properties object click on value selector (...) and from GT-SUITE Library select 'MaterialThermalProp' name it cordierite.



1.4 Surface Reaction Mechanism

- Primarily there are seven equations to calibrate, all the equations with respective parameters are represented in the table in slide4.
- From the library click on SurfaceReactions template and name it SCR_Mechanism. In the main tab for the species settings object creat translation choose the fluid reference object name for instance, o2-NASA, n2-NASA for the species name O2, N2 respectively. In the solver options the advanced adaptive is recomended for the efficient storage capabilities.
- Followed by, site element is Zeolite and the amount of loading is the active site density. Reaction rate equations templet is defined based on the Arrhenius general equation k = A*T^exp($\frac{-E_R}{RT}$)*(conc)^(cov)^[f(G)]

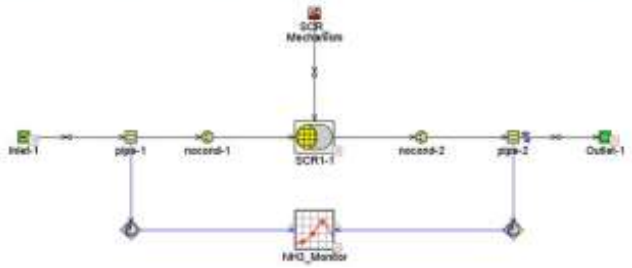


1.5 Monitor

- Monitor acts as a sensing device it dispalyes all the species signals from inlet and outlet. Drag and drop two 'def' SensorConn parts as shown in the figure below, in the composition set species mole farction and radio button click user-defined sensed species name, in the ... (three dots) library look for the species 'based on the requirements.
- From the Project Library doubleclick on the monitorsignal name as for example NH3 Monitor, drag the monitor to place on the main page and connect as shown in the figure.

1.6 Flow Connections

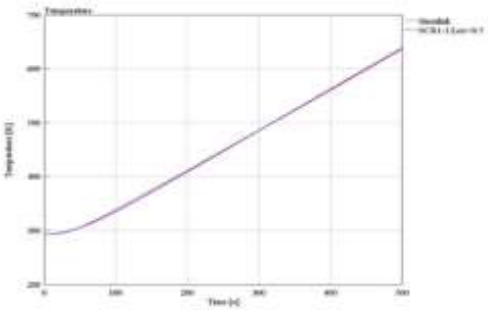
Finally, drag and drop components to main page to connect all the flow components, eventually the SCR model should look similar to the figure below.



Steps involved in SCR calibration methodology

1. Thermal Calibration

✓ The thermal properties of the SCR catalyst in GT must behave as that of the simulink block-box hence constant density is calibrated.



Inlet temperature in GT and Simulink

Time, sec	Temp, C
0	20
500	400

✓ Consider same inlet composition and temperature programmed desorption (TPD) profile in both GT and Simulink black-box

✓ Tune desity of the catalyst to match the thermal behaviour of the balck-box

Constant Conductivity	- W/(m-K)
Constant Density	- kg/m^3
Constant Specific Heat	- J/kg-K



2. Ad/Desorption Calibration

Step 1: Inlet section



- mass flow rate of the exhaust gas and constant temperature 200C, 300C, 400C and 500C or temperature programmed profile (TPD).
- Varied inlet ammonia composition with the amount of water and oxygen.
- Adsorption, desorption and oxidation equations are calibrated at the same time.



Step 2: Pipe

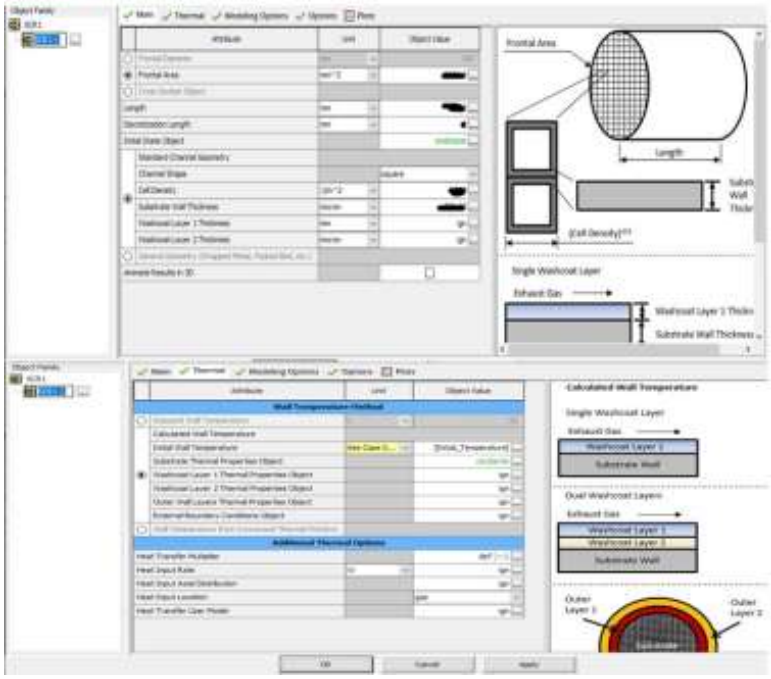


- The flow pipe between the inlet and SCR is adiabatic.
- Physical properties are as shown in the figure

GT-SUITE

GT-ISE

Step 3: SCR Catalyst



- Punch in the physical and thermal properties of the SCR
- For Ambstate pressure and temperature is as shown below



Attribute	Unit	Object Value
Pressure (Absolute)	bar	1
Temperature	See Case S...	[Initial_Temperature]
Composition		air-HASA

- For the substrate thermal properties object cordierite the constant conductivity, density and specific heat are refered to GT templet help.

GT-SUITE

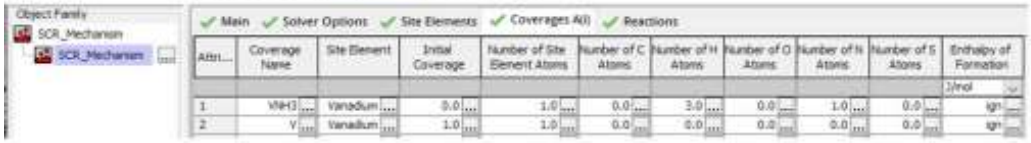
GT-ISE

Step 4: Surface Reaction Mechanism

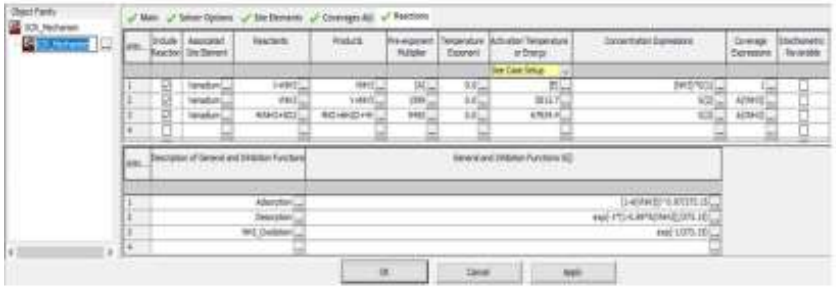


Attribute	Unit	1
Site Element Name		Vanadium
Site Density Option #1		
Active Site Density	mol/cm^3	[ActiveSiteDe...

- In the solver options tab select fixed mesh slover because of its robustness and it can be sloved to more discritization porosity in the catalyst.
- Site element is vanadium and it is a parameter in the storage calibration.
- In coverages tab, the number of atoms are menioned as show below.

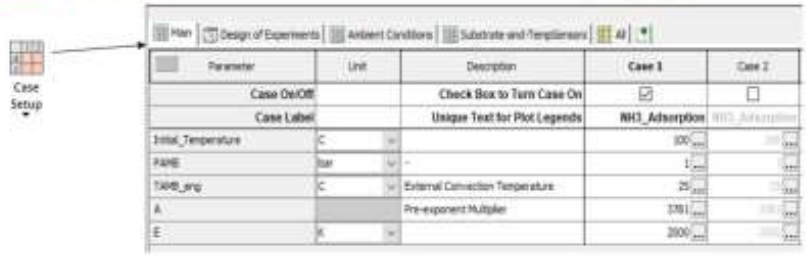


Attri...	Coverage Name	Site Element	Initial Coverage	Number of Site Element Atoms	Number of C Atoms	Number of H Atoms	Number of O Atoms	Number of N Atoms	Number of S Atoms	Enthalpy of Formation
										J/mol
1	VNH3	Vanadium	0.0	1.0	0.0	3.0	0.0	1.0	0.0	ign
2	V	Vanadium	1.0	1.0	0.0	0.0	0.0	0.0	0.0	ign



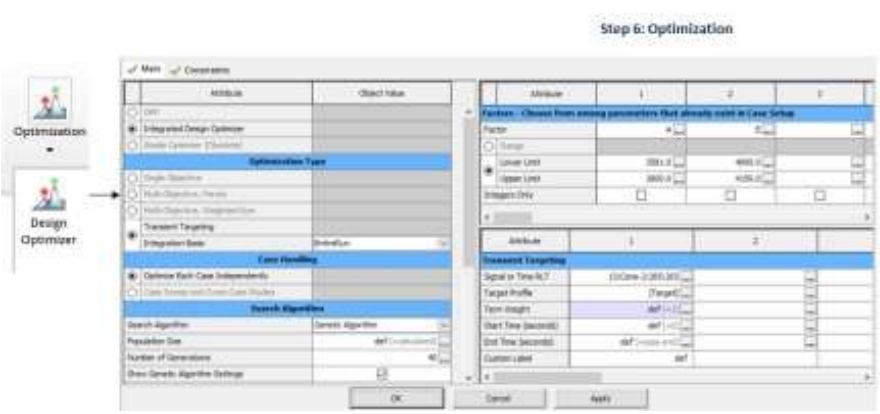
- In reactions tab, the representation of the Arrhenius reaction rate equation in GT is as shown in the adjacent shapshot.
- After the chemical connections between the components it is ready to run the model

Step 5: Case setup



- The attributes which changes continuesly are assigned as a parameter so that it can easely be changed in case setup

Step 6: Optimization



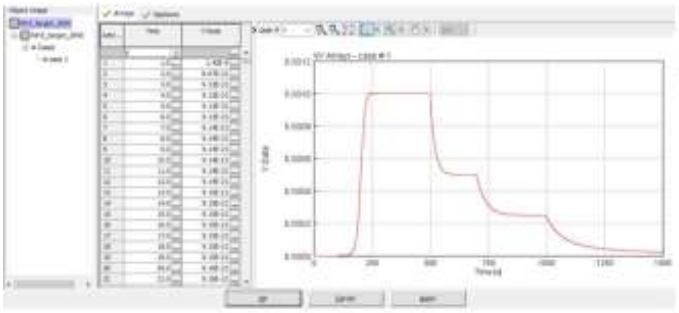
- Integrated design optimizer
- Use automatic design optimizer to iterate the paramers on targeting profile
- Here genetic algorithem is used as it is most widely used for the complex problems and sutable when there are two are more parameters to calibrate
- Number of generations are choosen
- Finaly, run the model with refrence A and E.
- Tune the parameters untill reach the target profile by running the model for number of iterations by both manual and automatic optimizer.

3. Oxidation Calibration

Step 1: Inlet Composition

- For the oxidation calibration the inlet composition ammona is supplied constant with some percentage of water and oxygen.

Step 2: Target Profile



- The target profile also varies as the inlet composition changes for oxidation so, from GT-library select ProfileTransient creat new object for example NH3_Target_200C here the array of time and mole fraction data is stored.
- Respective target profile is chosen in the case setup to run the optimizer. All the remaining setup is unchanged in the model and is redy to run.

4. DeNOx Calibration

- The inlet composition and target profile is replaced for the DeNox calibration.
- For the DeNox standard, fast and slow equations same calibration procedure is applied by adding the reaction rate equation in surface chemical mechanism.
- The procedure remains same for the remaning reaction equations i.e standard, fast and slow.