DISSERTATION

Modeling of Deposit Formation in SCR-Systems

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by

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Abstract

The permanently tightening emission regulations for nitrogen oxides pollutants force further development of mobile exhaust aftertreatment systems with selective catalytic reduction (SCR). Of particular interest is the long-term reliability of SCR systems with regard to unfavorable operating conditions, such as high injection rates of urea water solution (UWS) or low exhaust gas temperatures. Both may lead to the formation of solid deposits, which decrease system efficiency by increasing back pressure and impairing ammonia formation. A reliable numerical prediction of deposit formation in urea SCR systems is desired for the optimization of system design. However, comprehensive modeling of physical and chemical processes in the tailpipe, as well as the different time scale of involved phenomena, represents a challenging task.

To develop the required numerical approach, detailed experimental and numerical research on multiphase, reacting flows in SCR systems was performed. The most relevant processes of deposit formation were investigated at a wide range of realistic operating conditions using an optical box with heat-resistant glass inserted in the exhaust line of a diesel engine. The obtained experimental data provide a better understanding of spray/wall interaction, impingement heat transfer, the formation and propagation of liquid film, and the growth of solid deposits. Further, the experimental results were used to validate and extend the relevant numerical sub-models. The resulting simulation model was combined with a new source term approach to reduce the simulation run time.

The considerable speed-up of the Computational Fluid Dynamic (CFD) modeling made it possible to simulate several minutes of an experiment and thus take chemical reactions of deposit formation into account. Two different modeling approaches known from the literature were adapted to be integrated into the CFD code to predict solid by-product formation from wall films. The simulation results are in good agreement with the experimental data from the test bench regarding the position and composition of the deposits.

The current work also includes a modeling methodology for knitted wire mesh (WM) substrates, known for their great potential to reduce the deposit formation risk in SCR systems. Essential processes of spray/WM interaction, such as secondary droplet generation, wall film formation, and heat exchange, were analyzed in detail. A numerical model derived from basic measurements was set up in the following. The model was validated against experimental data and showed excellent results.

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Kurzfassung

Die Verschärfung der Grenzwerte für Stickoxidemissionen forciert die Weiterentwicklung von Abgasnachbehandlungssystemen mit selektiver katalytischer Reduktion. Von besonderem Interesse ist die langfristige Zuverlässigkeit von SCR-Systemen in Bezug auf ungünstige Betriebsbedingungen, wie hohe Einspritzraten der Harnstoff-Wasser-Lösung oder niedrige Abgastemperaturen. Beides kann zur Bildung von Feststoffablagerungen führen, die die Systemeffizienz durch Erhöhung des Abgasgegendrucks verringern und die Ammoniakbildung beeinträchtigen. Eine verlässliche, numerische Vorhersage der Ablagerungsbildung in SCR Systemen ist für die Optimierung des Systemdesigns wünschenswert. Jedoch stellt die umfassende Modellierung physikalischer und chemischer Prozesse im Auspuffrohr sowie deren unterschiedlichen Zeitskalen eine anspruchsvolle Aufgabe dar.

Um den erforderlichen numerischen Ansatz zu entwickeln, wurden detaillierte experimentelle und numerische Untersuchungen zu reaktiven, mehrphasigen Strömungen in SCR Systemen durchgeführt. Die wichtigsten Prozesse der Ablagerungsbildung wurden unter einem breiten Spektrum realistischer Betriebsbedingungen, mit Hilfe einer optischen Box mit hitzebeständigem Glas, untersucht. Die gewonnenen experimentellen Daten ermöglichen ein besseres Verständnis des Sprayimpingments, der Wärmeübertragung beim Aufprall, der Bildung und Ausbreitung des Flüssigkeitsfilms und des Wachstums der festen Ablagerungen. Darüber hinaus wurden die experimentellen Ergebnisse verwendet, um die relevanten numerischen Teilmodelle zu validieren und zu erweitern. Das daraus resultierende Simulationsmodell wurde mit einem neuen Quellterm-Ansatz kombiniert, um die Simulationslaufzeit zu reduzieren.

Die erhebliche Beschleunigung der CFD-Modellierung ermöglichte es, mehrere Minuten eines Experiments in einer Simulation zu modellieren und damit die chemischen Reaktionen der Ablagerungsbildung zu berücksichtigen. Zwei unterschiedliche aus der Literatur bekannte Modellierungsansätze wurden angepasst und in den CFD-Code integriert, um die Bildung von festen Ablagerungen aus Wandfilmen vorherzusagen. Die Simulationsergebnisse stimmen hinsichtlich der Lage und Zusammensetzung der Ablagerungen mit den experimentellen Daten überein.

Die aktuelle Arbeit umfasst auch eine Modellierungsmethodik für gestrickte WM-Substrate, die für ihr großes Potenzial zur Verringerung des Risikos der Ablagerungsbildung in SCR Systemen bekannt sind. Wesentliche Prozesse der Spray/WM-Interaktion, wie sekundäre Tröpfchenerzeugung, Wandfilmbildung und Wärmeaustausch, wurden detailliert analysiert. Infolge wurde ein numerisches Modell erstellt. Das Modell wurde anhand von Messdaten validiert und zeigte hervorragende Ergebnisse.

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Nomenclature

Latin Symbols

T_{crit}	°C	critical wall temperature
$\dot{m}_{crit}$	kg/h	critical injection rate

Chemical Compounds

CO_2	carbon dioxide
NO_X	nitrogen oxides
PM	soot particles
NH_3	ammonia
$(NH_2)_2CO$	urea
HNCO	isocyanic acid
H_2O	water

Abbreviation

CFD	Computational Fluid Dynamics
DOC	diesel oxidation catalyst
DPF	diesel particulate filter
EATS	exhaust aftertreatment system
ICE	internal combustion engine
IR	infrared thermography
KIT	Karlsruhe Institute of Technology
OP	operating point
RO	research object
SCR	selective catalytic reduction
TBU	thermal-induced breakup
TGA	thermogravimetric analysis
TL	Leidenfrost temperature
UWS	urea water solution
WM	wire mesh

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I. Introductory Chapter

The scientific and commercial projects I was involved in delivered valuable results in the modeling of deposit formation in SCR systems. Most results were published in scientific journal articles and project reports. Since the quality of my publications was recognized by experts, I was kindly given the opportunity to write my thesis as a cumulative dissertation following the guideline of TU Wien (see appendix). The main requirements for such dissertations are an introductory chapter, including the problem statement, the research objectives, methodology, the scientific contribution of the publication, and an enclosure of at least three peer-reviewed scientific journal articles.

1 Motivation

The transport sector, where internal combustion engines (ICE)s are presently dominant, faces worldwide ever more pressure to reduce greenhouse emissions by using sustainable energy. For instance, the EU commission has set ambitious targets to decrease carbon dioxide (CO_2) emissions of passenger and light-duty vehicles to at least 55 % below the 2021 level by 2030 [1]. In addition, a gradual reduction of CO_2 has been defined for new heavy-duty vehicles. The regulation EU 2019/1242 [2] obliges manufacturers to reduce their average fleet emissions by -30 % from 2030 onwards compared to a 2019-2020 monitoring period. Other countries such as the USA, Japan, and China are also aiming significant reduction of greenhouse emissions. Due to these facts, different scenarios are discussed in which the ICE-based powertrains will be replaced by battery electric vehicles. Figure 1 depicts an evolutionary powertrain scenario for the years 2021-2035 [3]. It is expected that the share of ICE-based powertrains will decrease by 64%, and the ICE will become increasingly part of hybrid powertrains.

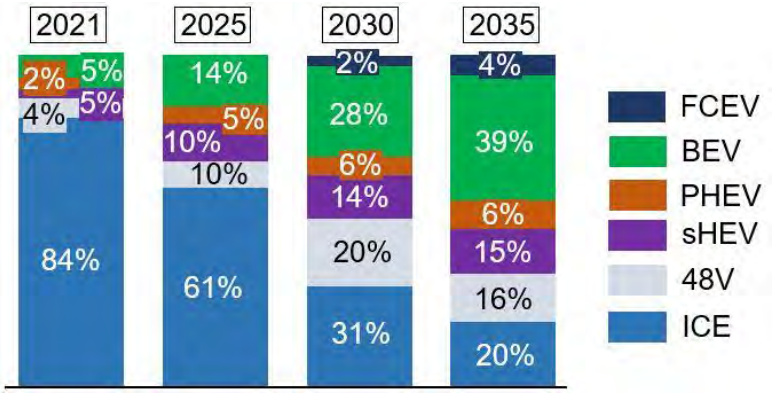

Figure 1: Evolutionary powertrain scenario for new sales of passenger and light commercial vehicles [3].

Many aspects of the generation and distribution of sustainable energy are not solved yet. Therefore, it is unclear whether the mentioned targets and scenarios will be fully met in the following decades. Nevertheless, it can be stated that the latest political

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decisions put enormous pressure on the producers of ICE-based powertrains to enhance overall system efficiency and enable a sustainable, CO_2-free engine operation.

Another significant challenge for the producers of ICE-based powertrains is fulfilling current and upcoming emission standards such as EURO VI and EURO VII. A general trend is the further tightening of regulation limits for nitrogen oxide (NO_X), soot particles (PM), carbon monoxide, and hydrocarbons and the introduction of additional limitations for ammonia (NH_3) and laughing gas emissions [4]. Moreover, the emission standards must be met under extended vehicle operating conditions with more durable exhaust aftertreatment systems (EATS)s. The temperature window of EATSs should be widened to lower and higher gas temperatures. The light-off of catalysts should be reached as fast as possible. These demands lead to the increased complexity of EATSs.

The rising pressure to operate the vehicles in an efficient and clean manner is a challenge for the future development of ICEs and EATS. Development methodology should provide cost-effective solutions within a short development timeframe despite the increasing demands. In this context, numerical methods are of particular interest for future development processes.

The present work deals with a numerical approach for the design optimization of UWS-based SCR systems. This kind of EATS has been and will remain an effective measure for reducing NO_X emissions from ICEs fuelled by diesel fuel and several renewable fuels such as hydrogen [5] or polyoxymethylene dimethyl ethers [6]. In particular, SCR systems will retain their importance for heavy-duty transports in the following decades. Due to the long driving distances, it is probably not efficient to defossilise this sector with electric vehicles alone [7]. The SCR technology offers engine manufacturers the possibility to overcome the well-known NO_X/efficiency trade-off. A higher acceptable amount of engine-out NO_X emissions enables a combustion process at the highest efficiencies, while SCR systems can accomplish the NOx limits.

The development of numerical methods for system optimization started simultaneously with the introduction of UWS-based SCR technology to the market. Nevertheless, there is still a need to improve the predictability of existing modeling approaches [8]. The modeling methodology should also be extended to simulate the formation of solid deposits, which are the most urgent problem of SCR systems at the moment. The following subsection provides an overview of processes happening within an SCR system and challenges for modeling methodology associated with these processes.

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2 Problem Statement

The NO_X-reduction in UWS-based SCR systems results from many complex physical and chemical processes. Figure 2 shows the most relevant processes and their time scales [9]. The reducing agent NH_3 is introduced in an SCR system with liquid UWS as a carrier fluid. For that, UWS is sprayed in the mixing section upstream of an SCR catalyst by a pressure-driven or air-assisted injector. While the first type is common for all applications of SCR systems, the last one can be found only in heavy-duty vehicles due to the availability of pressurized air. After injection, the UWS droplets propagate in the hot exhaust gas until they impact the system walls. The droplets may form a liquid film below the Leidenfrost temperature (TL). The high exhaust gas temperature causes fast dehydration of UWS in droplets and the liquid film. The remaining urea ($(NH_2)_2CO$) decomposes into ammonia and isocyanic acid (HNCO) in a thermolysis reaction [10–12], see Eq. (1). The released isocyanic acid gets further hydrolyzed to NH_3 and CO_2 in the SCR catalyst [13], as shown in Eg. (2). The highest possible ammonia production via reactions 1 and 2 is the most important development goal of current SCR systems.

$$(NH_2)_2CO \rightarrow HNCO + NH_3 \quad (1)$$

$$HNCO + H_2O \rightarrow NH_3 + CO_2 \quad (2)$$

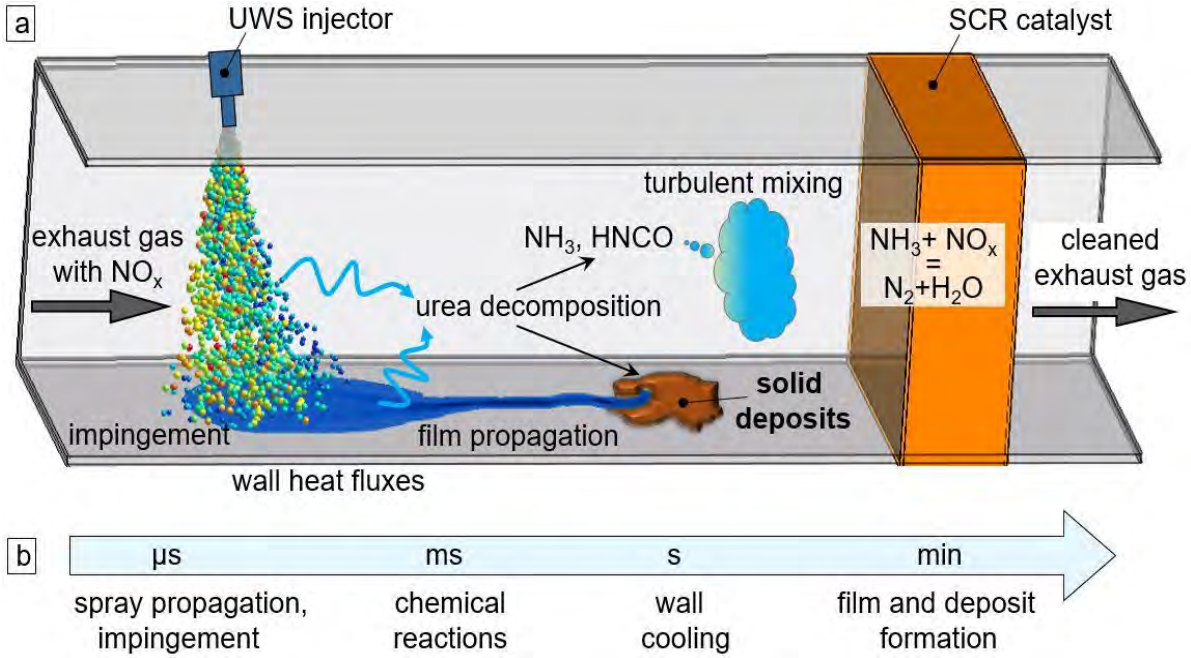

Figure 2: a - schematic overview of processes ongoing in an SCR system. b - overview of different time scales of relevant physical and chemical processes [9]

The turbulent gas flow transports the produced ammonia to the catalytic converter, where it reacts preferentially with NO_X due to the selective activity of the converter [14]. As a result, NO_X is reduced to elemental nitrogen. The optimal reduction is achieved by a homogeneous ammonia distribution in front of the SCR catalyst and uniform gas

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flow through the catalyst. Therefore, the efficient mixing of released ammonia with exhaust gas is significant for the SCR mixing sections. In this context, the word efficient also means a low pressure loss of the gas flow within a mixing section and a compact system design. The pressure loss should be kept as low as possible because it negatively affects the engine efficiency and thus the resulting CO_2 emissions. Compact design should ensure a simple and flexible integration of SCR systems in a vehicle.

Most manufacturers of SCR systems employ static mixing elements to enhance ammonia homogenization within the mixing sections. In recent decades a wide variety of mixer designs was proposed for SCR application: swirl, blade, plate, wire mesh mixer, among others. The mixers promote ammonia mixing with exhaust gas by increasing the turbulence in gas flow and, thus, the turbulent species transport. Moreover, sprays are usually targeted onto a mixing element. Droplet impingement on the mixer surface effectively shifts the original spray spectrum towards smaller diameters. That is beneficial for droplet evaporation and ammonia generation [15].

Under unfavorable operating conditions, such as a high injection rate of UWS or a low exhaust gas temperature, the initial footprint area of the spray can be significantly cooled down. That results in slow evaporation of the liquid film and, consequently, its accumulation. After a permanent liquid film is formed, it leaves the initial footprint area pushed by the shear stresses and gravity, as shown in Figure 2a. The film propagates toward regions with higher wall temperatures where the rate of urea decomposition accelerates again. Apart from the desired urea decomposition, several undesired side reactions may occur in the liquid film due to the high reactivity of isocyanic acid. The side reactions induce the formation of solid by-products of higher molecular weight, such as triuret, biuret, cyanuric acid, ammeline, ammelide, or melamine [10]. If the concentration of the by-products in the liquid film reaches a critical value, they stick to the walls of the mixing sections and block film propagation [9]. Further, the solid deposits start to grow. In contrast to spray injection and propagation which take place in time scales less than milliseconds, film and deposit formation occur in time scales of minutes, as shown in Figure 2b.

A high amount of accumulated solid deposits modifies the geometry of a mixing section and affects the gas flow field and spray/wall interaction. That increases back pressure in the system, decreases ammonia formation, and impairs its uniformity over the catalyst cross-section. Moreover, the corrosion of steel walls can appear near the formation area of deposits, leading to damage or even total failure of the SCR systems [16]. Depending on the deposit severity, deposits can be decomposed by increasing the exhaust gas temperature. Nevertheless, this possibility is limited under real driving conditions. The required decomposition temperature of some species, such as ammelide, ammeline, or melamine, is above 400 °C [10]. That is often well above the

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current exhaust gas temperature. Therefore, excessive deposit accumulation should be avoided to guarantee the reliable operation of SCR systems.

Applying a mixer element may considerably reduce the risk of deposit formation. A UWS spray targeted onto a mixer element produces a liquid film on a large surface area, increasing the heat flux from solid walls to the film and accelerating its evaporation [17]. Therefore, the risk of formation and propagation of a permanent liquid film, which is a precursor of deposit formation, can be shifted to higher injection rates. In particular, wire mesh mixers exhibit high resistance against deposit formation [18, 19]. The reason can be found in their large surface-to-volume ratio.

The design optimization of SCR mixing sections is a challenging task. The high performance and reliability requirements for mixing sections are often contrary to SCR systems' simple production and application. Numerous works in literature are devoted to the experimental optimization of mixing sections, e.g. [18, 20–22]. Considerable improvements in ammonia homogenization and reduction of deposit formation risk were achieved by performing cost and time-consuming experiments and adapting the system's components. Nevertheless, no universal design was proposed that would suit different applications of SCR systems. Instead, an optimum geometry of a mixing section and an injector concept should be found individually for every packaging requirement because it impacts the interaction of many physical and chemical processes.

The development methodology of SCR systems can be efficiently supported by numerical simulation. The CFD-based modeling provides a deep insight into the processes happening within a mixing section [15, 17, 23–25]. Thus, it helps to understand what design adaptations are necessary to improve the system efficiency. Moreover, exploration of different design parameters can be performed comparably faster and with lower effort. Nowadays, numerical methods are common in the development of SCR systems. Due to pressure on producers of SCR systems to ensure near-zero emissions of NO_x under real-world driving conditions, the need for fast, comprehensive modeling approaches is rising further.

Currently, numerical sub-models for modeling of physical processes, such as spray injection and propagation, droplet evaporation, turbulent mixing of ammonia, impingement, and film formation, are available. Based on them, modeling approaches for the prediction of ammonia uniformity in the front of an SCR catalyst were developed. Thus, an essential milestone in the developing methodology of SCR systems was achieved. The review article by Lauer [8] documents well the current status of the CFD-simulation method. Further, detailed kinetic models of urea decomposition were proposed containing thermolysis, hydrolysis, and reactions forming by-products [12, 26, 27]. The first simulations of deposit formation using these models were carried out,

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and promising results were obtained. Additionally, an alternative approach for predicting deposit formation based on the local properties of the liquid film was developed [17].

However, the predictability of some numerical sub-models, such as impingement models or impingement heat transfer models, should be improved [8]. Moreover, despite the experimentally proven great potential of WM mixers to reduce the deposit formation risk, the numerical approach for modeling of the spray interaction with the knitted WM structure is still missing. It is worth noticing that the interaction itself is not entirely understood.

The published results of ammonia homogenization and deposit formation modeling were limited to several seconds of real physical time due to high computational costs. The high effort can be attributed to numerous involved sub-models and different time scale phenomena (see Figure 2b), limiting the possible simulation time steps to approx. 0.1–1 ms [17, 28, 29]. In this regard, modeling of the spray propagation and the droplet impingement is most critical.

The inability to accomplish the modeling of liquid film and deposit formation with typical time ranges of several minutes is a significant drawback of available numerical approaches. The release of ammonia from a liquid film with a large spreading area differs significantly from the release predicted by a simulation during the first seconds. That may affect the quality of simulation results in terms of ammonia homogenization. Further, a physical time of several minutes should be simulated to precisely indicate the location and composition of solid deposits. Such simulation results have not been published yet, to the best of the author's knowledge. An effective speed-up method for simulation run time is required to eliminate the mentioned drawback.

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3 Research Objectives

The current work aimed to develop a comprehensive modeling approach for the prediction of deposit formation in UWS-based SCR systems in order to enable the effective optimization of the system's design and operating strategy. For this reason, all physical and chemical processes leading to the deposit growth on smooth steel walls of a mixing section had to be reproduced precisely. Typical time ranges of deposit formation had to be analyzed with an acceptable computational effort by adapting the simulation technique accordingly. The focus was put on deposit formation due to the UWS injection by pressure-driven injectors. Additionally, the approach had to include a modeling methodology for knitted WM substrates because of their known potential to reduce the deposit formation risk.

The defined aim was divided into several research objectives to facilitate its achievement:

- Profound knowledge of the underlying mechanisms of deposit formation had to be experimentally obtained. The impact of operating conditions on the deposit formation and decomposition had to be determined.
- A comprehensive experimental data basis with well-documented results had to be created for further validation of simulation models.
- Detailed insight into the mechanism of droplet-WM interaction had to be provided by experimental observations.
- Available numerical models of relevant physical sub-processes had to be revised and enhanced, if necessary.
- A speed-up method for substantial reduction of simulation run time had to be established.
- The available chemical kinetic model by Brack [26] and the alternative modeling approach by Smith [17] had to be integrated into the used CFD code and validated against measurement data.
- An empirical model derived from basic measurements had to be developed to cover the impact of the WM substrate on an SCR system. An appropriate modeling approach was missing.
- The developed comprehensive modeling approach had to demonstrate the capability to predict the location and composition of solid deposits for a wide range of operating conditions.

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4 Methodology

Experimental and numerical research was carried out to achieve the defined objectives. In the following subsections, the applied research methods are explained in detail. It starts with experimental investigations divided into experiments performed on engine and component test benches.

4.1 Experimental research

4.1.1 Investigation on Engine Test Benches

The formation of solid deposits within a mixing section of an SCR system results from many physical and chemical processes running simultaneously. The most important of them are:

1. generation of UWS spray
2. spray evaporation
3. spray propagation
4. spray impingement
5. wall cooling
6. liquid film formation and its propagation
7. reactions of urea decomposition
8. growth of deposits

The goal of experimental research was to provide a detailed understanding of processes 3 – 6, 8 and create a good basis for further validation of numerical models. Another objective was to study the severity of existing deposits and the possibility of removing them.

Experimental study of deposit formation and decomposition within a real mixing section is difficult due to the limited access of the measurement instruments. Therefore, appropriate test benches were designed [16, 30], as shown in Figure 3. They provided enough space for different measurement techniques and reproduced deposit formation at conditions similar to a real SCR system. The main components of the test benches are a supplier of the exhaust gas and an optical box, as shown in Figure 3a. A turbocharged heavy-duty diesel engine supplied clean exhaust gas to the optical box with desired temperature and mass flow rate. The optical boxes enabled optical access to research objects (ROs) placed inside. Various operating conditions and spray properties were used to obtain a comprehensive data basis, as shown in Figure 4. Chosen operating points (OP)s are typical for low, medium, and high load points of a diesel engine and cause different liquid film and deposit formation mechanisms. The spray properties have a high impact on impingement regimes and wall cooling [9]. Due to the extensive experimental matrix, the gained knowledge from experiments can be

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transferred to real SCR systems with different designs and possible operating conditions.

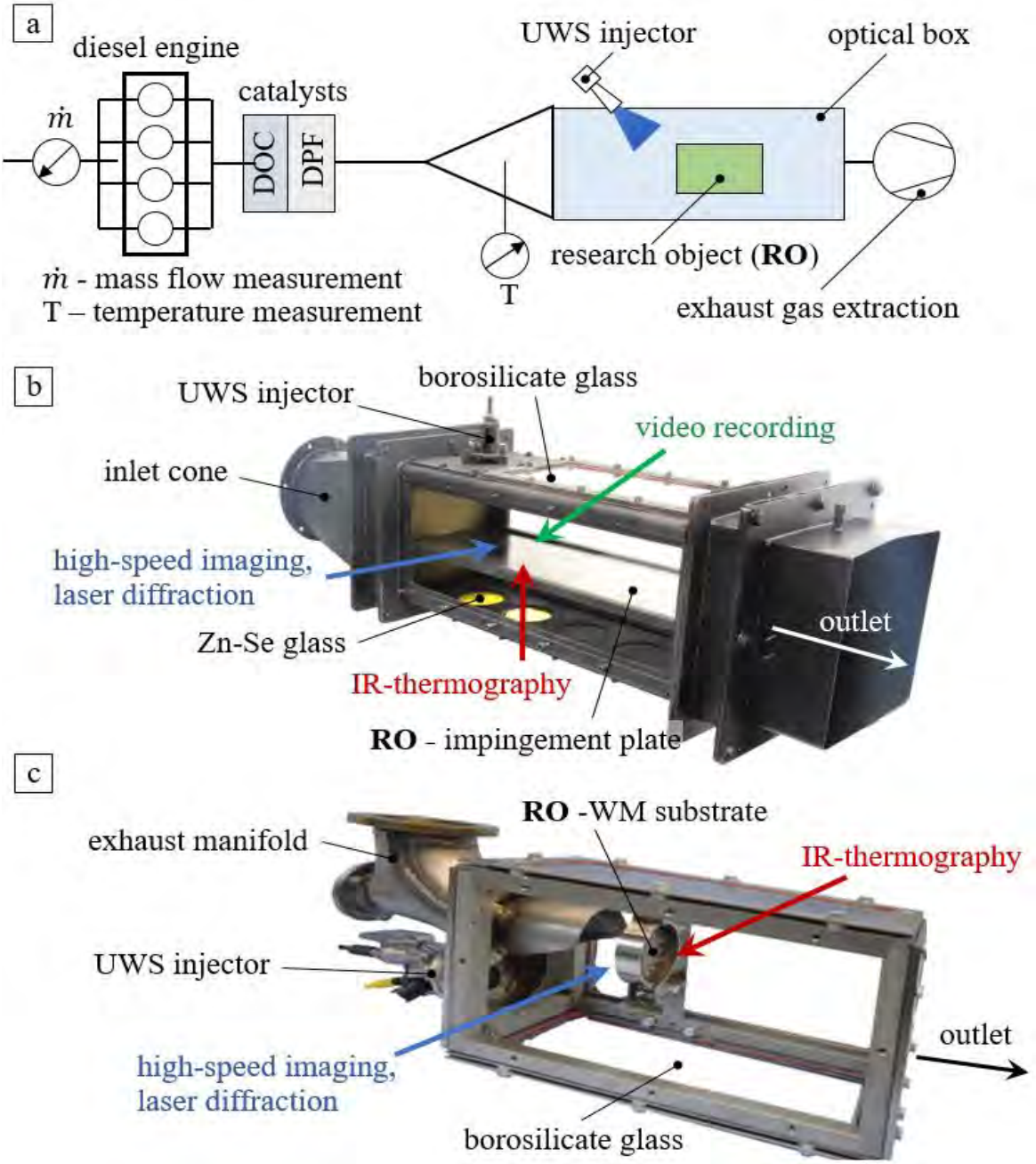

Figure 3: a - Schematic layout of the engine test bench. b – optical box for investigation of deposit formation and decomposition on the impingement plate, c – optical box for investigation of WM substrate.

The setup shown in Figure 3b used an impingement plate as a RO. The generated experimental results are characteristic for spray impingement, film, and deposit formation on smooth steel walls of an SCR mixing section. Furthermore, this setup enabled the investigation of spray propagation, which significantly impacted the processes mentioned above. The trajectories of droplets within the gas flow are determined by their initial momentum and forces acting on them. According to the

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literature [31], the drag force is the most dominant force in typical SCR systems. The critical parameter for its modeling is the drag coefficient. The Schiller-Naumann correlation [32] of the drag coefficient is often used in CFD codes. The measurement results of the laser diffraction method and high-speed imaging were used to validate this correlation, as described in [9]. Specification of employed measurement techniques is summarized in Table 1. The initial spray momentum of used injectors was found with the help of component test benches, as explained in the following subsection.

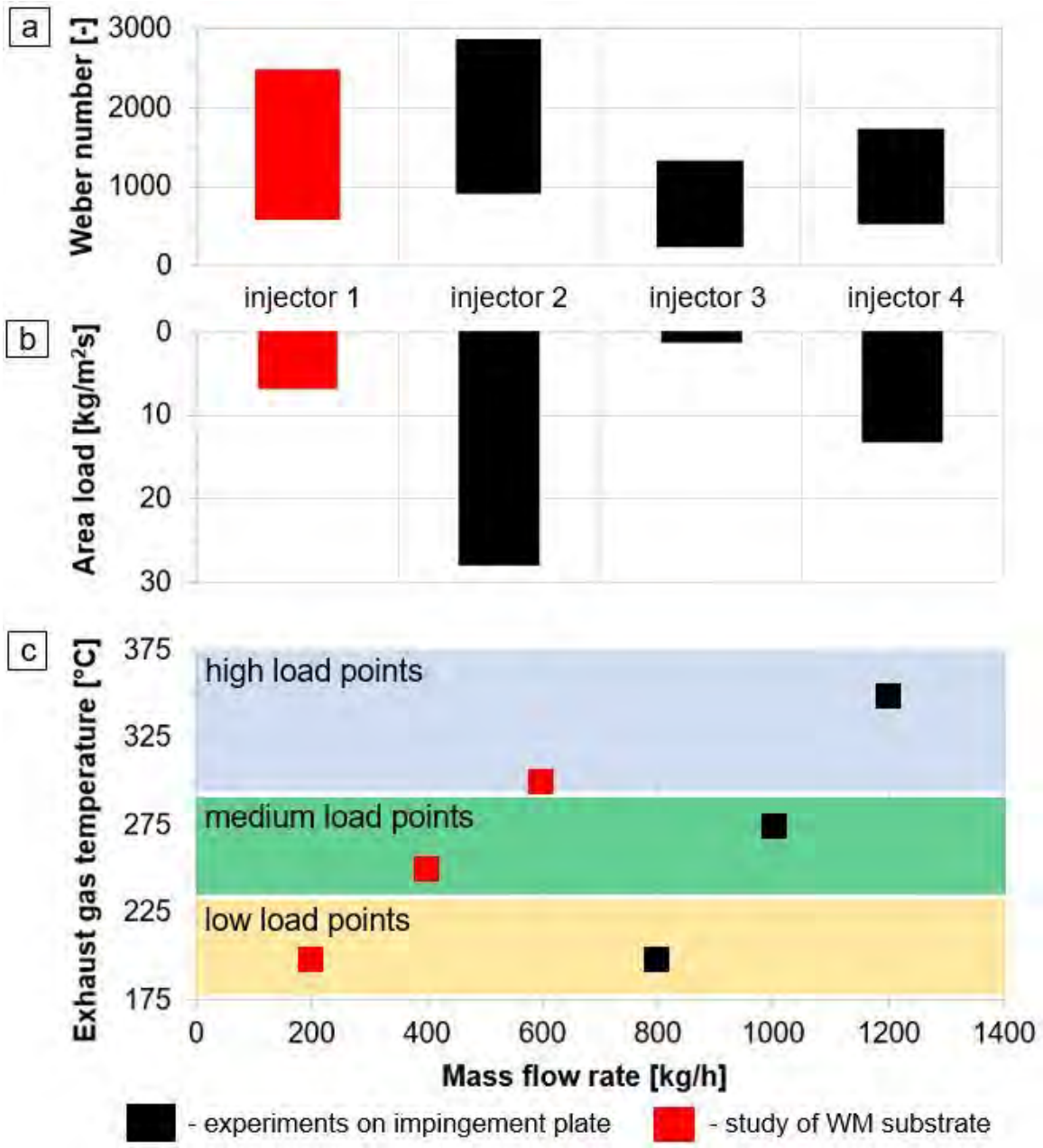

Figure 4: Operating conditions and injectors properties used to investigate the impingement plate and WM substrate. a – range of Weber numbers calculated with the initial spray velocity for droplet spectrum between Dv10 and Dv90. b – area load of used injectors at the distance of 50 mm from the injector tip. c – operating points.

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Table 1: Applied measurement techniques

Technique	Documentation of	System	Specification
high-speed imaging	• initial velocity and geometry of spray • spray propagation	PCO Dimax HD	• frame rate 3 kHz • exposure time 2 µs
laser diffraction	• droplet size distribution in spray	SprayTec	• diameter of the laser beam 10 mm • measurement frequency 2.5 kHz • measurement duration 10 s
video recording	• formation of liquid film and solid deposits • high-resolution imaging of WM	Canon EOS 650D	• resolution of video 1920x1080 pixel • frame rate 24 Hz • resolution of 5184x3456 pixel
(IR)infrared thermography	• material temperature	ThermoIMAGER TIM 640	• temperature range from -20 to 900 °C • framerate of 32 Hz • resolution of video 640x480 pixel
thermogravimetric analyser (performed by KIT)	• composition of solid deposits	Netzsch STA 409 C	• temperature range from 40 to 700°C • heating rate of 2 K/min • synthetic air • flow rate of 100 ml/min

Spray impingement on a solid wall is a precursor of liquid film and deposit formation at unfavorable operating conditions. It is a complex issue influenced by multiple parameters: incident spray characteristics, physical properties of the wall and its temperature, surface properties such as roughness, coating, or surface impurities (e. g., soot). Depending on mentioned parameters, different impingement regimes are possible [25, 33–35]. The following quantitative values characterize the result of an impingement regime: the intensity of impingement heat transfer, mass fraction of an

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incident droplet that remained on the surface, the impulse to the liquid film, the size distribution of the secondary droplets, and their velocities. The most popular numerical models of UWS spray impingement [35, 36] require empirical correlations to calculate these values.

To validate these correlations, spray impingement below and above the Leidenfrost temperature (TL) was documented. The plate cooling by the spray was measured by an IR camera through zinc selenide windows. The results revealed a dependency of TL on the incident droplet Weber numbers. A corresponding correlation was deduced [23]. Furthermore, the temperature drop of the plate during impingement above the TL is a measure of the intensity of the impingement heat transfer. Therefore, the measured data were used to validate Wruck's impingement heat transfer model [37]. The temperature drop for impingement below the TL correlates with the mass fraction of spray that remained on the plate as liquid film and further evaporated [38]. The size distribution of secondary droplets produced below and above the TL was measured with the help of the laser diffraction method. The results highlighted that in contrast to the impingement above the TL, the secondary droplet spectra below the TL are nearly independent of the incident spray properties [16]. That indicated that most secondary droplets were ejected from the liquid film using the thermal energy of the solid wall.

For investigation of film propagation and deposit formation, a high injection rate of used injectors was set at different load points of the diesel engine. That provoked the accumulation of permanent liquid film in the initial spray footprint and its further spreading downstream the gas flow. Video recording revealed different propagation types of the film: wave motion of thick film, small rivulets, and sliding of large droplets [16]. The type of film propagation substantially impacted the contact area between the film and the wall, the heat exchange between them, and consequently, the spreading area of the film. The solid deposits were created from the liquid urea wherever the film stagnated. The growth of solid deposits and the wall temperature in the area of their formation were observed by the video and IR cameras, respectively. The composition of produced deposits was determined with the help of the thermogravimetric analyzer at KIT, as described in [16].

The same setup was used to investigate the mechanisms of deposit decomposition. Of particular interest were possibilities to remove previously generated solid deposits by changing operating conditions. The impact of the increased exhaust gas temperature and the mass flow rate was studied independently. For that reason, in the first part of the experiments, a noticeable amount of deposits was generated. After that, the UWS injection was stopped, and one of the mentioned parameters was rapidly changed while maintaining the other. The measurement techniques were applied similar to the investigation of deposit formation. The results revealed that in contrast to

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the increased mass flow rate, the rise of the exhaust gas temperature has a great potential to remove solid deposits from an SCR-System. Additional experiments were performed to study the spray interaction with solid deposits. The operating conditions were changed to overlap the initial spray footprint with the position of previously produced deposits. An eroding of the solid deposits by the spray was observed.

A WM mixer is a specific part of some SCR systems that has a complex interaction with UWS spray in terms of droplet breakup and wall film formation. The test bench setup shown in Figure 3c was developed to study these processes. The position of WM substrate, 90° manifold, and injectors is typical for off-road exhaust systems. Care was taken to keep the gas flow upstream of the WM undisturbed and at the same time provide enough space for measurement technique. The laser diffraction method was applied to investigate the droplet impingement up and downstream of the WM substrate. The comparison of obtained droplet spectrums revealed the intense production of small droplets within the substrate. The high-speed imaging clarified the interaction of the spray with the wires. The events of droplet splash, rebound, deposition, and transition were observed. The infrared thermography was used to monitor the wetting of WM surface due to the impingement regime "deposit." The observation showed the strong ability of the WM mixer to evaporate the wall film from its large surface. The knowledge obtained from the measurement campaign was used to develop and validate the new numerical model of droplet WM interaction.

4.1.2 Investigations at Component Test Benches

Lab test benches shown in Figure 5 were developed to investigate previously mentioned UWS injectors under ambient conditions. The goal was to determine initial spray properties: droplet velocity, droplet size distribution, static mass flow rate, and spray geometry. The obtained data served to initialize sprays in CFD simulations using the Lagrangian approach. The spray geometry and initial droplet velocity were determined with the help of the high-speed camera, as shown in Figure 5a. The spray was prepared by a UWS injector and the universal dosing system. The dosing system provided the injector with the necessary mass flow rate and pressure of UWS. It also controlled the injectors in terms of injection frequency and injection time. UWS was sprayed between the light source and the high-speed camera. A high light intensity enabled the camera to produce a series of images with a short exposure time of 2 µs and a frequency of 3000 fps. The propagation velocity of droplets near the injector tip and the spray geometry were determined using the images' spatial resolution and the recording's temporal resolution.

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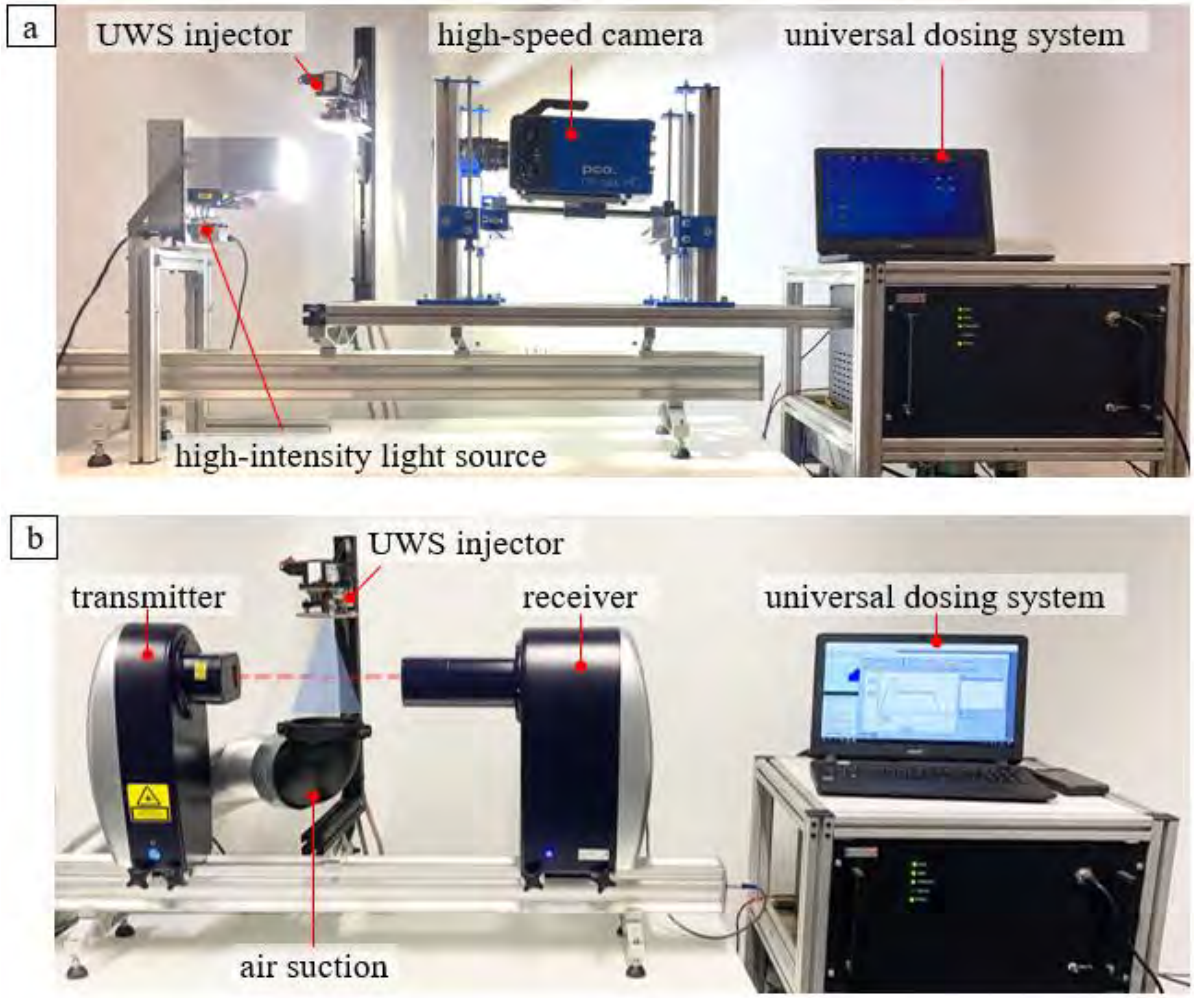

Figure 5: Test bench setups for determination of spray characteristics. a – high-speed imaging of UWS spray. b – measurement of droplet size distribution in a spray.

Figure 5b depicts the experimental facility designed to measure droplet size distribution in a spray. The measurement instrument includes the transmitter and receiver module. The transmitter produces a laser beam with a diameter of 10 mm. During the measurement time of 10 seconds, it passes through the spray cone with a frequency of 2,5 kHz. Droplets scattered the light from the beam inversely proportional to their size. The scattering pattern from the spray is captured by detecting optics in the receiver module. The pattern is further analyzed, and the time-averaged droplet size distribution is calculated. The choice of the measurement position in the spray is critical concerning the output result. On the one hand, most droplets of a spray cone should intersect the laser beam. Therefore, the closest measurement position to the injector tip is desired. On the other hand, a spray should be fully developed at this place. To satisfy both conditions and thus find optimal measurement positions, the results of high-speed imaging were used. The distance from the release point of an injector to the optimal measurement position varied between 20-30 mm for investigated injectors.

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An important question is whether the droplet size distribution measured under ambient conditions can be used for spray initialization in CFD simulations at different OPs. To find out the answer, the droplet size distribution was measured in the hot, calm exhaust gas. The optical box was conditioned to the temperature of an OP. After that, the engine was stopped, and the measurement was performed. Figure 6 provides an exemplary comparison of droplet spectra of the injector №4 measured at 20 °C and 275 °C. The presented spectra are nearly congruent. The results also indicate that the borosilicate glass did not affect the measurement process.

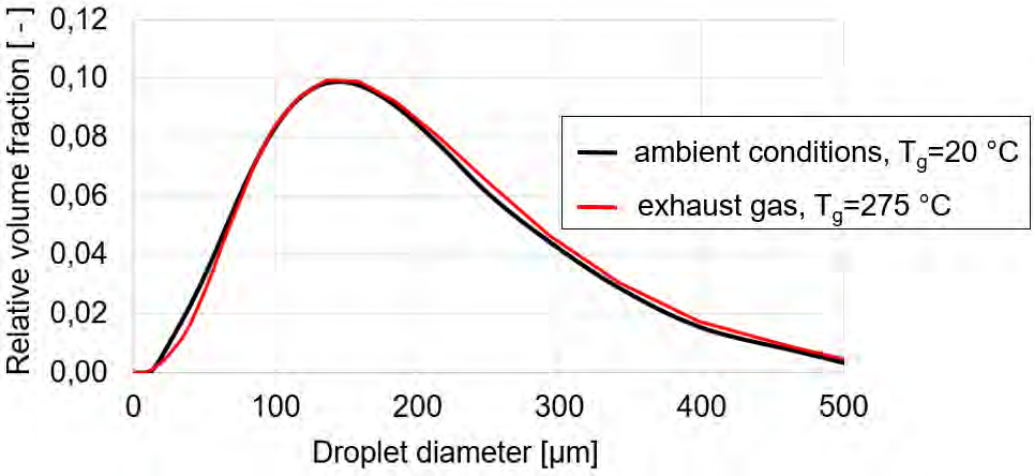

Figure 6: Comparison of droplet spectra measured under ambient conditions and at exhaust gas temperature of 275 °C.

It must be emphasized that the accuracy of measured data was of major importance for basic research. The investigation on the injector test bench showed that the measured initial spray properties could differ considerably from the data provided by manufacturers. The reason may lie in the production tolerances of injectors and the usage of different fluids for the measurement of spray properties.

For modeling of WM mixers, a new modeling approach was developed. It is based on the probability of interaction between a droplet and the WM. The probability was found with the help of a high-resolution image recorded using the test bench setup shown in Figure 7a. The WM was placed between the light source and the camera to avoid the shade of wires on the obtained images. Additionally, a white light dispersing foil was located between the light source and the WM. These measures provided a clear contrast between black pixels of the WM and white pixels of the background, as shown in Figure 7b. The camera was placed 1,2 m away from the WM. On the one hand, it reduced the perspectival distortion of the images. On the other hand, the distance was not too far to have a high image resolution of 50 pixels per 1 mm. Based on the obtained image, the impingement probabilities of UWS droplets with WM were analytically determined, as explained in the following section.

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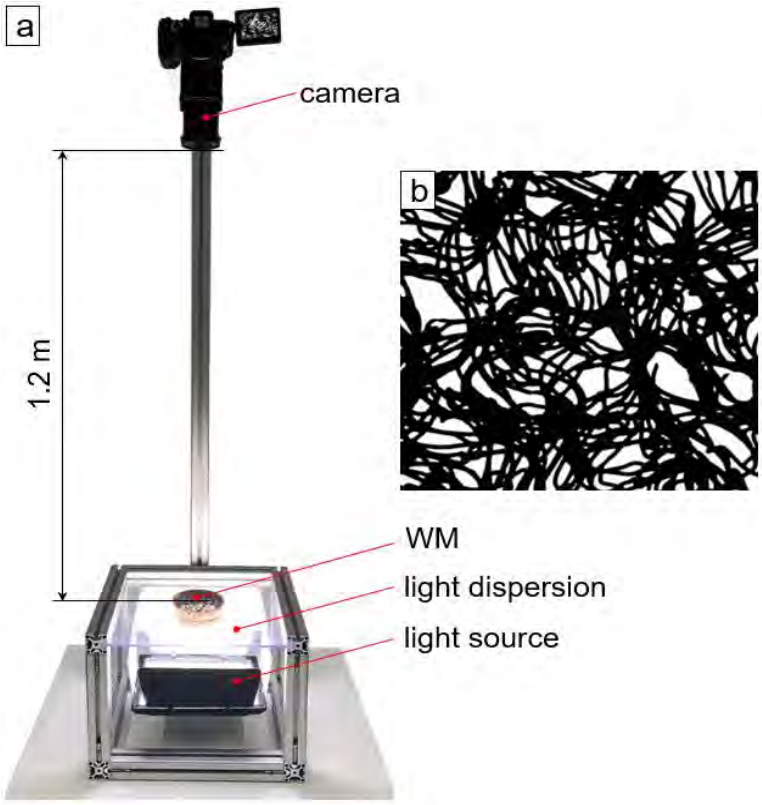

Figure 7: a - Test bench for making high-resolution backlight images of WM substrates. b – part of the obtained image.

4.2 Numerical research

The ultimate goal of numerical research was to develop a comprehensive simulation approach for modeling of deposit formation. It had to comprise detailed numerical sub-models and deliver meaningful simulation results within reasonable computation time. The numerical research was carried out with the help of commercial CFD-code Star-CCM+ v.1306. However, the developed modeling methodology is not specifically designed for this code and allows its implementation in other suitable simulation environments.

Numerical modeling of deposit formation can be partitioned into two steps: modeling physical processes from the UWS injection to the formation of liquid film and modeling chemical reactions within the liquid film. The CFD modeling approach proposed by Fischer [15] was used in this work as a basis for modeling physical processes. It embraces turbulent flow, spray, and film formation and demonstrated good simulation results concerning the prediction of the ammonia uniformity. Nevertheless, the most critical sub-models had to be revised and validated. The order of model validation is important and was strictly followed, as shown in Figure 8.

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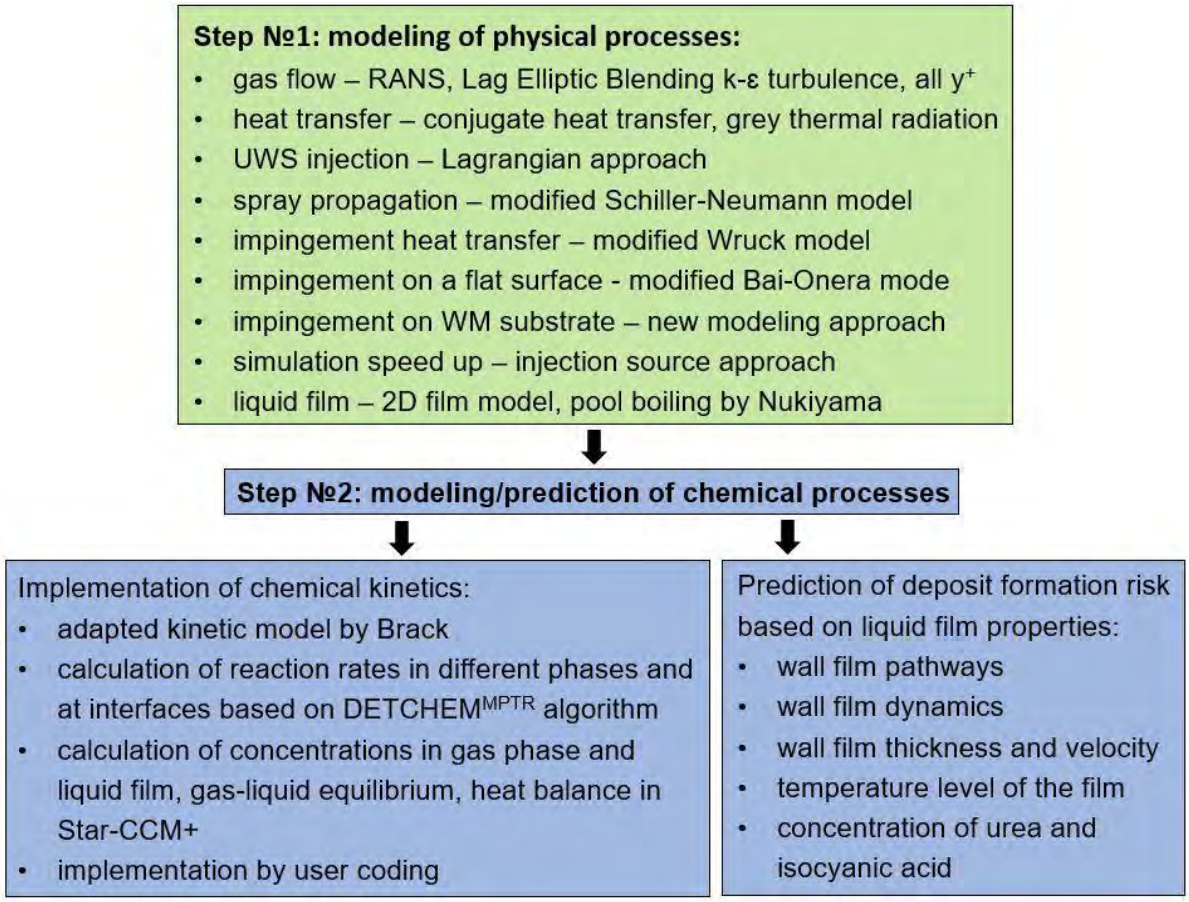

Figure 8: CFD-modeling of physical and chemical processes involved in deposit formation in SCR system

The modeling of the turbulent gas flow is placed on the top of the validation hierarchy because it impacts all following sub-processes. Different turbulence models were compared, and the Lag Elliptic Blending *k*-ε realizable model was chosen for further numerical research. Due to its high accuracy in near-wall regions, the heat transfer between the gas flow and solid walls was well captured. Furthermore, experimental observations revealed that thermal radiation might play an essential role in heat transfer between solid walls. Therefore, the gray thermal radian and surface-to-surface radiation models were included in the CFD modeling. The simulated temperature field prior to the UWS injection matched the measurement results excellently [24]. That was the necessary condition for further successful validation of spray and film models.

For modeling the UWS sprays, a multiphase Lagrangian approach was used that involves a high number of numerical parcels to represent a spray. After initializing Lagrangian particles in the CFD code, each parcel's momentum equation is solved to predict their motion. The change in momentum is balanced by forces that act on the droplet. The drag force is most dominant in typical SCR systems. One of the standard Lagrangian drag coefficient methods, Schiller-Naumann correlation, was applied for its modeling. The validation of this correlation against the measured data revealed the overestimation of the drag coefficients for droplets with a size range of 25-300 μm.

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Therefore, the original correlation was modified with the Cunningham correction factor to fit the experimental results [9].

The next step in the validation hierarchy was the revision of numerical models describing the spray-wall interaction. The most advanced and flexible impingement model Bai-Onera and impingement heat transfer model by Wruck were chosen as a basis for impingement modeling. Comparison of obtained simulation and experimental results revealed the need to enhance them when dealing with realistic UWS sprays [8]. First of all, no distinct TL, as initially set in the Bai-Onera model and proposed by other authors [25, 29, 35, 36], could be experimentally observed. Instead, investigations showed a dependency of TL on the incident droplet Weber numbers [16]. An empirical correlation hat to be deduced and implemented in the CFD code to cover this phenomenon [23]. Further, the experimental investigations showed a smooth transition between the Leidenfrost effect and wall wetting by a spray. The mass fraction of incident droplets remaining on the wall as a film increased gradually with the drop of the wall temperature. The key model parameters had to be adjusted to match these experimental observations. Moreover, the thermal-induced breakup (TBU) impingement regime had to be added to the model, similar to the proposal by Quissek [34]. The model by Wruck initially developed for fuel sprays was also modified to get satisfactory results for UWS spray. In particular, the model parameters describing the droplet deformation during their impact on a wall were adjusted to count the physical properties of UWS [23].

By contrast to the impingement on a flat surface, no modeling methodology was available for spray interaction with a WM substrate. A detailed representation of the WM structure in a CFD model is not practicable due to its complex and not fully determined geometry. Therefore, a new empirical model derived from basic measurements was developed [30]. A conventional porous medium was introduced in the CFD model instead of the detailed geometry of WM. The defined properties of this medium take the back pressure of the WM into account and reproduce the droplet impingement on the structure that appears with a certain probability. A MATLAB algorithm was developed to calculate the impingement probability based on the high-resolution image of the WM substrate. A multi-regime impingement model was set up to model possible impingement events. The experimental results of the laser diffraction method and infrared thermography were used to adjust the impingement model.

The validation of drag force and impingement modes revealed that the presence of Lagrangian parcels in the simulation domain limited the maximal simulation speed by approx. 2 s per day using one computer core per 35,000 cells. The modeling of numerical parcels increased the simulation time for a time step up to 100 %. Moreover, it limited the maximal possible time step by approx. 1 ms due to stability problems. The short steps did not allow film and deposit formation modeling with a typical time range of several minutes. Therefore, a new speed-up method called "injection source

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approach" was proposed [24]. In this method, the source terms of mass, momentum, and energy substituted the numerical parcels representing the spray. The application of source terms allowed to increase the simulation time steps up to 10 ms.

Since simulations with a long time duration became possible, the second step in the simulation of deposit formation – modeling of chemical reactions was carried out. As shown in Figure 8, two different modeling approaches known from the literature were applied. The first approach employs a chemical solver for quantitative modeling of deposit formation. The kinetic model suggested by Brack et al. [26] and extended by Börnhorst et al. [9] was adapted to integrate it into the CFD code via a user code. The second approach allows qualitative prediction of deposit severity and deposit location based on liquid film properties, as proposed by Smith et al. [17]. Major influence factors promoting or impeding deposit formation were revised with the help of the detailed experimental results from the optical box. Furthermore, a more precise definition of the initial spray footprint could be introduced thanks to the mentioned injection source approach. Thus, the overall accuracy of the method was improved.

To demonstrate the capability of developed comprehensive modeling approaches, deposit formation was conducted within the optical box and a real SCR system of a heavy-duty diesel engine. The reliability of simulation results was evaluated for different conditions of the exhaust gas flow and the spray properties. The results showed good agreement with the experimental observations regarding the wall cooling, deposits' position, and composition. Nevertheless, some disadvantages of the used 2D film model were discovered. The model does not capture the effect of the surface tension that leads to the overprediction of the width of the film front. Furthermore, the model is not suitable for the modeling of thick liquid films.

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5 Summary of the Research Results

5.1 Summary of peer-reviewed publications

Table 2 provides an overview of peer-reviewed publications required by the guideline of TU Wien for cumulative dissertations (see appendix). The table also shows the shares of contribution.

Table 2: overview of peer-reviewed publications

№	Publication
1	Budziankou, U., Quissek, M., Lauer, T.: **Deposit Formation in SCR-Systems - Optical Investigations**; SAE International Journal of Advances and Current Practices in Mobility 3(1), p. 501-515, 2021; doi:10.4271/2020-01-2177
	85 % authorship; performing, analysis and scientific documentation of all experiments except for the thermogravimetric analysis.
2	Budziankou, U., Quissek, M., Lauer, T.: **A Fast Modeling Approach for the Numerical Prediction of Urea Deposit Formation**; SAE International Journal of Advances and Current Practices in Mobility 2(3), p. 1337-1355, 2020; doi:10.4271/2020-01-0358
	85 % authorship; performing, analysis and scientific documentation of all experiments except for the thermogravimetric analysis, validation and enhancement of numerical submodels, enhancement of the modeling approach by Smith.
3	Budziankou, U., Börnhorst, M., Kuntz, C., Deutschmann, O., Lauer, T.: **Deposit Formation from Urea Injection: A Comprehensive Modeling Approach**; Emission Control Science and Technology, 6 (2): p. 211-227, 2020; doi:10.1007/s40825-020-00159-x
	45 % authorship; performing, analysis and scientific documentation of all experiments except for the thermogravimetric and high-performance liquid chromatography analysis, development of the speed-up method, integration of kinetic model by Brack
4	Budziankou, U., Lauer, T., Yu, X., Schmidt, B. et al.: **Modeling Approach for a Wiremesh Substrate in CFD Simulation**; SAE Technical Paper 2017-01-0971, 2017; doi:10.4271/2017-01-0971
	80 % authorship; high-speed imaging of spray impingement, determination of impingement probability, analysis of all measurements data, development and validation of the modeling approach.

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Publications 1 - Deposit Formation in SCR-Systems - Optical Investigations

This publication deals with an experimental study of the most relevant physical processes of deposit formation in UWS-based SCR systems. These include spray impingement on a hot surface, wall cooling, liquid film formation, liquid film propagation, and growth of solid deposits. Additionally, the paper describes possibilities to remove accumulated solid deposits in a typical SCR system. The impact of changing operating conditions on deposit decomposition was presented.

To study the deposit formation under realistic conditions, an engine test bench was developed. Solid deposits were generated under stationary operating conditions. Three different commercial injectors were used for spray generation at every OP. The experiments at the high OP showed a strong impact of spray properties on the critical wall temperature T_{crit} and the critical injection rate $\dot{m}_{crit}$. These values determent the transition between the Leidenfrost effect and the beginning of wall wetting by a spray. With the help of IR measurements, it was found that sprays with a low area load and low Weber numbers have high values of $\dot{m}_{crit}$ and T_{crit}. Furthermore, measurements based on the laser diffraction method demonstrated the importance of the TBU impingement regime. This regime governed the appearance of secondary droplets after an impingement event in the temperature range from approx. 160 °C up to T_{crit}. Therefore, the droplet spectra produced in this temperature range were almost equal and seemed not to depend on the sprays' initial properties.

Video recording of the liquid film at different OPs revealed four types of its possible propagation: thin liquid film, thick liquid pool, rivulets, and large droplets. The kind of film propagation affected the distance at which a liquid film could spread from the initial impingement area and thus the final position of solid deposits. They were produced wherever the film stagnated. The minimal wall temperature that triggered the formation of solid deposits was found to be approx. 200 °C. The composition of solid deposits was analyzed with the help of thermogravimetric analysis (TGA) at Karlsruhe Institute of Technology (KIT). The relation between the temperature of the liquid film and the composition of solid deposits was determined based on these analyses.

The deposit decomposition was observed under transient operating conditions. The impact of the mass flow rate and the exhaust gas temperature was determent. In contrast to the increased mass flow rate, the rise of the exhaust gas temperature has a great potential to remove solid deposits from an SCR System. Furthermore, a new mechanism of deposit removal by spray was observed. It was found that solid deposits were effectively removed wherever their position overlapped with the impingement area of the spray.

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Another only rarely documented undesired side-effect of the permanent wall wetting was discovered. The permanent hot liquid film triggered steel corrosion. Based on the IR-measurement results, the critical film temperature of approx. 235 °C was found. The corrosion speed of the impingement plate was estimated to be 0.45-0.65 mm/day.

Finally, the relevance of gained knowledge was explained concerning the operating strategy of an SCR system and modeling of deposit formation with the help of CFD tools. To achieve more realistic modeling, several improvement requirements were pointed out. They include the necessity to accomplish the modeling of deposit formation within the time of several minutes, accurate modeling of spray impingement within a wide range of wall temperatures, the need to model different types of film propagation, and the application of a detailed chemical solver for modeling of side reactions of urea decomposition.

Publication 2 - A Fast Modeling Approach for the Numerical Prediction of Urea Deposit Formation

The paper describes a methodology for modeling of the deposit formation risk. Its main advantages are high simulation speed and a simple application. The improvement requirement of CFD tools to accomplish the modeling of several minutes was successfully achieved. The proposed approach does not model any side reactions of urea decomposition, and thus, it does not require any chemical solver. Instead, deposit formation risk is predicted based on the properties of the liquid film.

Another essential part of this publication deals with the accurate modeling of spray impingement. For that reason, experimental data mentioned in the first publication were analyzed, and several modifications of a suitable impingement model were made to fit the experimental observations. The available Bai-Onera model [39] was chosen as a basis for impingement modeling. It was changed for its use with UWS sprays. The initial key parameter that determent the regime transition was adapted. Furthermore, the model was modified concerning the definition of T_{crit}. It was expressed as an empirical function of the We-number. In addition, similar to the work published by Quissek et al. [34], the TBU impingement regime was added to the model. A correlation for a droplet mass remaining on the wall as the film was found. For modeling of the impingement heat transfer above T_{crit} an adapted model proposed by Wruck [37] was used. The droplet deformation in this model was adjusted with the Akao correlation.

A new method called "injection source approach" was developed to speed up the CFD simulation. In this approach, numerical parcels were substituted by source terms of mass, momentum, and energy. They were calculated simultaneously during the first injection event, stored, and applied to the film and gaseous phase in the following injection events. The substitution of the numerical parcels had a double positive effect:

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on the one hand, it reduced the numerical effort, and on the other hand, it allowed to increase the simulation time step. The new modeling approach was validated against the measurement results from the optical box, which were obtained for two different UWS injectors and two OPs. Simulation results correlated well with the IR-thermography in temperature ranges below and above TL. Also, the transition from no wall wetting to liquid film formation was well reproduced by the simulations. That is a confirmation of the accuracy of developed and modified models.

For modeling of deposit formation risk, the approach by Smith et al. [17] was used. The original approach was modified based on experimental observations from the optical box. The critical values of film velocity and minimal film thickness were adapted. Thanks to the injection source approach, a new determination of the initial footprint was introduced. The modified modeling approach was validated against the experimental data from the optical box and a real SCR system. The simulation results showed a good agreement with the experimental data regarding the expected composition of solid deposit and their location. Moreover, the simulation predicted the appearance of rivulet within the mixing section of the real SCR system.

The main disadvantage of the approach is the impossibility to model deposit decomposition. Therefore, this approach cannot be used for modeling of transient operating conditions where deposit decomposition is possible. However, it is well suited for fast estimating of deposit formation at steady-state OPs. Based on the obtained results, a preselection of systems with the best designs can be carried out.

Publication 3 - Deposit Formation from Urea Injection: A Comprehensive Modeling Approach

This publication deals with the modeling of deposit formation and decomposition at steady-state and transient operating conditions. It differs from the previous publication in using of a kinetic model for modeling of side reactions of urea decomposition. The modeling approach was also modified to consider a higher number of film and gas components. The kinetic model by Brack et al. [26] served as the basis for the description of chemical reactions. It was extended by Börnhorst et al. [9] with thermodynamic equilibria between the different phases (gaseous, liquid, solid) and adapted for the integration into CFD code. To solve possible chemical reactions in the liquid film, the software package Detchem [39] was used. It was implemented into CFD code through a user-coded interface. The data of concentrations, temperature, and pressure in the film were transferred from the CFD code to the user code for each cell and in each time step. The user-coded algorithm calculated reaction rates. The resulting production terms were transferred back into CFD code to update the species concentrations in the liquid film.

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The experimental data from the optical box at two different OPs were used to validate the simulation results. The first experiment was carried out at a steady-state operating condition with an exhaust gas temperature of 350 °C. The first three minutes of the experiment could be simulated. During this time T_{crit} was reached, and spray started to form a liquid film which propagated downstream the exhaust gas flow. Due to the high temperature of liquid film side reaction of urea decomposition was triggered. The formation of biuret and ammelid was predicted by the chemical solver. During the simulation time, the liquid film's thickness reached a critical value of 400 µm. Further modeling was not possible because the film thickness got equal to the thickness of the first prism layer in the fluid region. Simulation residuals showed solution divergence. The inability to model a thick liquid film was an essential disadvantage of the used 2D-liquid film model. Nevertheless, the comparison of measured and simulated results during the first three minutes showed the capability of the modeling approach to predict the position and chemical composition of solid deposits.

The second experiment was conducted at transient operating conditions. Solid deposits were produced during the first 5 minutes of the experiment at the exhaust gas temperature of 275 °C. After that, UWS injection was stopped, and deposit decomposition was observed during the second part of the experiment. The remained deposits were analyzed using TGA and high-performance liquid chromatography at KIT. The experiment could be simulated completely because the liquid film did not reach the critical value. The comparison of simulated and measurement results showed that the wall cooling by the spray and position of solid deposit was well predicted during the whole simulation time. Nevertheless, some inaccuracies in the modeling of film spreading and decomposition of solid deposits were discovered. The reasons for that were analyzed, and improvements were suggested. They include using more advanced 3D-liquid film models such as "Volume of fluid model [40]" or a hybrid film model [40] and implementing an improved kinetic model. Furthermore, the necessity of more accurate modeling of liquid film tension and viscosity was pointed out.

Publications 4 - Modeling Approach for a Wiremesh Substrate in CFD Simulation

This peer-reviewed publication describes the modeling methodology of WM mixers used as additional parts of SCR systems. Several experimental studies proved their efficiency in reducing the formation of solid deposits. However, the implementation of a WM in CFD modeling was difficult due to its complex geometry. Therefore, an alternative modeling approach hat to be developed.

As the first step, the interaction processes between a WM substrate and both UWS spray and exhaust gas flow were investigated experimentally. High-speed videography was used to identify the impingement regimes. The droplet spectrum upstream and

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downstream of the WM was measured using the laser diffraction method. Infrared thermography was applied to investigate WM cooling by the spray. The experimental findings provided a detailed insight into the mechanism of droplet WM interaction. The experiments showed that the WM effectively promoted droplet breakup. A lot of small secondary droplets were detected downstream of the subtract. Due to the large surface-to-volume ratio of the WM, fast film evaporation from its surface was observed.

Based on gained knowledge, an empirical modeling approach was proposed. The WM mixer was handled as a conventional porous medium that takes the back pressure of the substrate into account. The complex interaction of the spray with the WM was reproduced with the help of porous baffles defined within the porous medium. The droplets could interact with these virtual surfaces in the form of discrete events: transmit, rebound, deposition, and splash. The probability of interaction between a droplet and the WM was determined as a function of the droplet diameters, which was found based on a high-resolution image of the substrate. For modeling of impingement regimes, an existing impingement model was adapted. The model parameters were adjusted to fit the experimental observations. The evaporation rate of the droplets chosen by the model to stick on the WM was estimated based on the IR measurements. The developed modeling approach reproduced well the main characteristics of the WM substrate.

5.2 Summary of additional publications

Table 3 provides an overview of not peer-reviewed publications.

Table 3: overview of not peer-reviewed publications

№	Publication
5	Börnhorst, M., Budziankou, U., Kuntz, C., Lauer, T.: **Fundamental Experimental and Numerical Investigation on the Deposit Formation and Decomposition from AdBlue in SCR-systems**; Final report of the FVV project no. 1262 "AdBlue Deposits"; 2019: https://www.fahrzeugindustrie.at/fileadmin/migrated/news_uploads/FVV_H1191_V1262_AdBlue_Deposits.pdf
	45 % authorship; performing of the experiments with the engine test bench, modeling of spray propagation, impingement, film formation and propagation, development of the speed-up method.
6	Budziankou, U., Kuntz, C., Börnhorst, M., Lauer, T.: **Investigations on the Deposit Formation and Decomposition from Urea in SCR Systems**; MTZ Worldwide, Vol. 82, p. 62–65, 2021; doi:10.1007/s38313-020-0589-8
	45 % authorship; writing of the publication based on the final report of the FVV project.

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Publication 5 - Fundamental Experimental and Numerical Investigation on the Deposit Formation and Decomposition from AdBlue in SCR-systems

This work is the final report of the FVV research project number 1262, "AdBlue deposits". The report was not peer-reviewed but was presented to the expert audience of the project. It is available for all FVV members and the members of “Fachverband der Fahrzeugindustrie Österreichs”. The TU Wien and the KIT performed the project to develop a comprehensive modeling approach of UWS decomposition and deposit formation. The report describes all research activities carried out to reach the project goal in detail. It served as the basis for creating of publications 1-3.

In addition to the publications mentioned above, the report includes validation results of the drag force model. For that purpose, the spray deflection by the gas flow in the optical box was documented with the help of high-speed imaging and laser deflection methods. The measurements were conducted at three different OPs and with three UWS injectors to generate a dataset sufficient to validate simulation results. The validation of the spray deflection showed an over-estimation of the drag coefficients of the droplets within a size range of 25-300 µm. Therefore, the used drag coefficient was modified to reduce the drag force for small droplets.

Publication 6 - Investigations on the Deposit Formation and Decomposition from Urea in SCR Systems

This not peer-reviewed publication in MTZ worldwide journal describes the research results of the FVV project "AdBlue Deposits" shortly. It is based on the final report of this project. It is intended for the professional public, which may be interested in comprehensive modeling of deposit formation and decomposition in automotive SCR systems. The MZT worldwide journal greatly impacts the technology-oriented management in the automotive industry with a particular focus on engine development.

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6 Scientific Contribution of the Dissertation

The scientific contributions of this work can be summarized as follows:

- New scientific findings of sub-processes of deposit formation are obtained
  - The impact of droplet diameters in the range of 10 – 300 µm on the drag force is precisely identified.
  - The dependency of the critical wall temperature on spray properties is determined.
  - Different types of liquid film propagation and their impact on the location of deposit formation are discovered.
- The severity of solid deposits at different operating conditions is evaluated.
- The effect of changing operating conditions on deposit decomposition is assessed.
- A comprehensive modeling approach for the prediction of deposit formation is proposed
  - Numerical sub-models of spray propagation and impingement are modified and extended.
  - A new speed-up method for substantial reduction of simulation run time is presented.
  - Modeling approaches from the literature were adapted and enhanced to integrate into the CFD code.
- A detailed insight into the mechanism of droplet/WM interaction is provided.
- A modeling methodology for WM substrates in CFD simulation is developed.

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8 Appendix

Richtlinie des Vizerektors für Lehre über die Verfassung von kumulativen Dissertationen an der Technischen Universität Wien

Auf Grundlage von § 19 Abs. 2 Z 1 Universitätsgesetz 2002- UG (BGBI. I Nr. 120 idgF.) iVm. § 1 der Studienrechtlichen Bestimmungen der Satzung der Technischen Universität Wien sowie § 82 UG wird vom Vizerektor für Lehre verordnet:

Präambel

Diese Richtlinie ergänzt die Regelungen über das Verfassen einer Dissertation im Doktoratsstudium gemäß § 23 der Studienrechtlichen Bestimmungen der Satzung der Technischen Universität Wien (idF. des Senatsbeschlusses vom 27. Juni 2011).

§1

Vereinbarung einer kumulativen Dissertation

Eine Dissertation ist im Regelfall als Monographie zu verfassen. Im Einvernehmen zwischen der Doktorandin/dem Doktoranden und der Betreuerin/dem Betreuer (im Falle einer Ko-Betreuung im Einvernehmen mit allen Betreuenden) kann mit Zustimmung der zuständigen Studiendekanin/des zuständigen Studiendekans auch die kumulative Form vereinbart werden.

§2

Zusammensetzung einer kumulativen Dissertation

(1) Eine kumulative Dissertation hat im Regelfall mindestens drei publizierte oder angenommene wissenschaftliche Aufsätze in international anerkannten wissenschaftlichen Zeitschriften oder Büchern mit wissenschaftlichem Lektorat, die einem Peer-Review-Verfahren unterzogen wurden, zu enthalten.

(2) Bei Ko-AutorInnenschaften ist der Beitrag der Doktorandin bzw. des Doktoranden im einleitenden Kapitel der Dissertation (§ 3 Abs. 1 Z 1) präzise darzulegen. Ein und dieselbe Publikation mit mehreren Autorinnen kann nur mit Zustimmung der Studiendekanin bzw. des Studiendekans Bestandteil von mehr als einer kumulativen Dissertation der TU Wien sein.

(3) Der kumulativen Dissertation ist ein Einleitungskapitel vorangestellt. In diesem Kapitel sind der Zusammenhang der Publikationen und die Einordung in das jeweilige Fachgebiet darzustellen.

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§3

Struktur einer kumulativen Dissertation

(1) Die kumulative Dissertation besteht aus

1. dem einleitenden Kapitel und
2. den wissenschaftlichen Aufsätzen.

(2) Das einleitende Kapitel hat

1. die Problemstellung,
2. die Ziele,
3. die Methodologie,
4. eine kurze Zusammenfassung der wissenschaftlichen Aufsätze sowie
5. den wissenschaftlichen Beitrag der Dissertation

zu enthalten. Die Nachvollziehbarkeit der Resultate muss aus der Beschreibung der wissenschaftlichen Methodologie eindeutig hervorgehen.

§4

Beurteilung und Einreichung einer kumulativen Dissertation

(1) Die Beurteilung einer kumulativen Dissertation erfolgt gemäß § 23 der Studienrechtlichen Bestimmungen der Satzung der TU Wien sowie gemäß den jeweils geltenden Bestimmungen des Studienplans für das Doktoratsstudium der Naturwissenschaften/Sozial- und Wirtschaftswissenschaften/Technischen Wissenschaften an der TU Wien.

(2) Die Einreichung und Abgabepflicht einer kumulativen Dissertation erfolgt nach den Bestimmungen der Richtlinie über die elektronische Abgabepflicht von Hochschulschriften (Mitteilungsblatt 14-2013 idgF.). Die elektronische Version einer kumulativen Dissertation hat das einleitende Kapitel (§ 3 Abs. 1 Z 1) und abweichend vom gedruckten Exemplar lediglich die Literaturzitate der wissenschaftlichen Aufsätze (§ 3 Abs. 1 Z 2) zu enthalten.

§5

Inkrafttreten

(1) Diese Richtlinie tritt nach Veröffentlichung im Mitteilungsblatt der Technischen Universität Wien mit 1. Oktober 2013 in Kraft.

(2) § 1 in der Fassung Mitteilungsblatt 2014, 15. Stück, Nr. 165, tritt mit 1. Oktober 2014 in Kraft.

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9 Curriculum Vitae

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Academic Career

10/2015 - present	**Vienna University of Technology** Doctoral Programme in Engineering Sciences Institute for Powertrains and Automotive Technology Project Assistant
8/2012 - 05/2015	**University of Stuttgart** Master's Diploma in Automotive and Engine Technology
9/2005 - 6/2010	**Belarusian National Technical University** Master's Diploma in Engine Technology

Professional Career

10/2015 - present	**Vienna University of Technology** Institute for Powertrains and Automotive Technology Project Assistant
9/2011 - 9/2012	**Minsk Wheel Tractor Plant Open Joint Stock Company** Ladder frame development Development engineer

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II. Published Work

1

Budziankou, U., Quissek, M., Lauer, T.: **Deposit Formation in SCR-Systems - Optical Investigations**; SAE International Journal of Advances and Current Practices in Mobility 3(1), p. 501-515, 2021; doi:10.4271/2020-01-2177

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Budziankou, U., Quissek, M., Lauer, T.: **A Fast Modeling Approach for the Numerical Prediction of Urea Deposit Formation**; SAE International Journal of Advances and Current Practices in Mobility 2(3), p. 1337-1355, 2020; doi:10.4271/2020-01-0358

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3

Budziankou, U., Börnhorst, M., Kuntz, C., Deutschmann, O., Lauer, T.: **Deposit Formation from Urea Injection: A Comprehensive Modeling Approach**; Emission Control Science and Technology, 6 (2): p. 211-227, 2020; doi:10.1007/s40825-020-00159-x

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Budziankou, U., Lauer, T., Yu, X., Schmidt, B. et al.: **Modeling Approach for a Wiremesh Substrate in CFD Simulation**; SAE Technical Paper, 2017; doi:10.4271/2017-01-0971

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