CFD Simulation of Urea Evaporation in STAR-CCM+

Master Thesis - Report

Oscar Ottosson
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Academic supervisor: Magnus Andersson
Industrial supervisors: Emma Alenius, David Norrby
Examiner: Roland Gårdhagen
Abstract

Diesel engines produce large amounts of nitrogen oxides ($NO_X$) while running. Nitrogen oxides are highly toxic and also contribute towards the formation of tropospheric ozone. Increasingly stringent legislation regarding the amount of nitrogen oxides that are allowed to be emitted from diesel-powered vehicles has forced manufacturers of diesel-engines to develop after-treatment systems that reduce the amount of nitrogen oxides in the exhaust. One of the main components in such a system is selective catalytic reduction (SCR), where nitrogen oxides are reduced to diatomic nitrogen and water with the help of ammonia. A vital part of this process is the spraying of a urea-water-solution (UWS), which is needed in order to produce the reducing agent ammonia. UWS spraying introduces the risk of solid deposits (such as biuret, ammelide and ammeline) forming in the after-treatment system, should the flow conditions be unfavourable. Risk factors include high temperatures, but also low dynamics and high thickness of the resulting liquid film that forms as the UWS spray hits the surfaces of the after-treatment system. It is thus essential that manufacturers of SCR after-treatment systems have correct data on how much UWS that should be sprayed into the exhaust for any given flow condition. Experimental tests are thoroughly used to assess this but are very expensive and are thus limited to prototype testing during product development. When assessing a wider range of concepts and geometries early on in the product development stage, simulation tools such as computational fluid dynamics (CFD) are used instead.

One of the most computationally heavy processes to simulate within a SCR after-treatment system is the UWS spray and its interaction with surfaces inside the after-treatment system, where correct prediction of the formation of solid deposits are of great importance. Most CFD models used for this purpose hold a relatively good level of accuracy and are utilized throughout the whole industry where SCR aftertreatment is applied. Despite this, these models are limited in the fact that they are only able to cover timescales in the scope of seconds to minutes while using a tolerable amount of computational power. However, the time spectrum for solid deposit formation is minutes to hours.

Scania is one of Sweden’s biggest developers of SCR after-treatment, with the technology being incorporated directly into its silencers. AVL Fire is the main UWS spray simulation tool for engineers at Scania at the moment. One major drawback of using AVL Fire for UWS spray simulations is that it is deemed too time-consuming to set up new cases and too unstable during simulation, which makes it too costly in terms of expensive engineering hours.

This project has investigated the potential of using STAR-CCM+ for UWS spray simulations at Scania instead. A standard method has been evaluated, as well as parameters that will prove useful in further investigations of a potential speedup method. The studied method in STAR-CCM+ is easy to setup and the simulation process is robust and stable. Various other perks come from using STAR-CCM+ as well, such as: a user-friendly interface, easy and powerful mesh-generation and
great post-process capabilities.

Several different parameters have been investigated for their impact on the studied method, such as mesh refinement of the spray injector area and the number of parcels injected every time-step through the spray injector (simply put the resolution of the spray). A possible speedup by freezing the momentum equations when allowed and lowering the amount of inner iterations has also been investigated.

A handful of operating conditions have been studied for two different geometries. The attained simulation results display correlations with physical measurements, but further assessment for identifying the risk of solid deposit needs to be performed on the studied cases to assess the full accuracy of solid deposit prediction of the studied method. Recommendations for future work include fully implementing and evaluating the speedup method available for spray simulations in STAR-CCM+ as well as directly comparing how the accuracy and performance of the method relates to that of the method used in AVL Fire for spray simulations.
Sammanfattning


En av de mest beräkningsstunga processerna att simulera i ett efterbehandlingssystem med SCR är sprayandan av urea-lösning och dess interaktion med ytor, där korrekta förutbestämmelser av huruvida det finns risk för klumpbildning eller inte är av stor betydelse. De flesta CFD modeller som används i detta syfte har förhållandevis god noggrannhet och används i stor utsträckning i den bransch där efterbehandling med SCR tillämpas. Däremot är dessa modeller begränsade i att de endast kan åstadkomma simulerningar (med en acceptabel mängd datorkraft) som sträcker sig i tidsintervall sekunder till minuter. Bildningen av klump är dock en process som kan ta upp till flera timmar.

Scania är en av Sveriges största tillämpare av SCR, då tekniken används i de efterbehandlingssystem som finns inbyggda i tillverkarens ljuddämpare. Scania använder främst AVL Fire för simulering av spray med urea. AVL Fire anses dock vara för tidskrävande vid skapelsen av nya simuleringssfall och för instabilt under simulering.

Detta projekt har därför undersökt möjligheten att använda STAR-CCM+ för simulering av spray med urea hos Scania. Den metod i STAR-CCM+ som utvärderats är enkel att använda då nya simuleringsfall ska skapas, samtidigt som den är robust och stabil under simulering. Relevanta parametrar för en potentiell uppsnabbningsmetod har också undersömts. STAR-CCM+ i sin helhet är användarvänligt, där verktyget för att skapa och generera mesh är enkelt att använda såväl som kraftfullt när mer avancerade operationer krävs. Möjligheterna för post-processing är väldigt smidiga för transenta förlopp, vilket är ett stort plus för simuleringar med
urea-spray, vars injektion och resulterande processer är väldigt transienta skeenden i sig.

Flera olika parametrar har undersökts, för att granska hur stor påverkan de har på prestandan och noggranheten hos den studerade metoden. Två av dessa är tätheten av beräkningsnoder i den region där spray-munstycket är placerat samt antalet paket med urea-vatten lösning som injiceras varje tidssteg via spray-munstycket. En möjlig uppsnabbning av metoden, som går ut på att frysa ekvationerna för bevarelse av rörelsemängd (eng - momentum equations) när det är tillåtet och samtidigt minska antalet inre iterationer för varje tidssteg, har också undersökt.

Acknowledgements

Firstly, I would like to thank Kim Petersson, Head of the Fluid Dynamics and Acoustics Simulation team (NXPS) at Scania, for the great opportunity to work on this project. It has been a treasured experience to work at NXPS, where I have learned a whole lot about CFD simulations and their application in the transport industry.

I want to give heartfelt thanks to my supervisors at NXPS, Emma Alenius and David Norrby, for providing guidance, feedback and support throughout the whole project.

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I thank Fredrik Thelin for his great work involving physical tests and post-processing of the Large silencer.

I thank Louis Carbonne at NXPS, who has provided great insight and theoretical knowledge into the subject of spray simulations.

I thank Constantine Nottbeck for his important contributions on physical tests and simulations of the Akvariet geometry.

I want to thank Rodolfo and Christian from the support team at Siemens for STAR-CCM+, for their great support and insightful answers regarding STAR-CCM+.

Lastly, I would like to acknowledge the contributions from the Parallel Computing Center (PDC) at KTH, whose resources and support have proved invaluable for the simulations performed throughout this project.
Nomenclature

Abbreviations and Acronyms

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Meaning</th>
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<tbody>
<tr>
<td>LiU</td>
<td>Linköping University</td>
</tr>
<tr>
<td>KTH</td>
<td>Royal Institute of Technology</td>
</tr>
<tr>
<td>CFD</td>
<td>Computational fluid dynamics</td>
</tr>
<tr>
<td>CAD</td>
<td>Computer aided design</td>
</tr>
<tr>
<td>CPU</td>
<td>Central processing unit</td>
</tr>
<tr>
<td>PDC</td>
<td>Parallelldatorcentrum (Center for High Performance Computing)</td>
</tr>
<tr>
<td>DES</td>
<td>Detached Eddy Simulation</td>
</tr>
<tr>
<td>LES</td>
<td>Large Eddy Simulation</td>
</tr>
<tr>
<td>UWS</td>
<td>Urea Water Solution</td>
</tr>
<tr>
<td>SCR</td>
<td>Selective catalytic reduction</td>
</tr>
<tr>
<td>DOC</td>
<td>Diesel oxidation catalyst</td>
</tr>
<tr>
<td>DPF</td>
<td>Diesel particulate filter</td>
</tr>
<tr>
<td>ASC</td>
<td>Ammonia slip catalyst</td>
</tr>
<tr>
<td>DOE</td>
<td>Design of experiments</td>
</tr>
</tbody>
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Chemical formulas

<table>
<thead>
<tr>
<th>Formula</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>CO</td>
<td>Carbon monoxide</td>
</tr>
<tr>
<td>CO₂</td>
<td>Carbon dioxide</td>
</tr>
<tr>
<td>CO(NH₂)₂</td>
<td>Urea</td>
</tr>
<tr>
<td>H₂O</td>
<td>Water</td>
</tr>
<tr>
<td>HNCO</td>
<td>Isocyanic acid</td>
</tr>
<tr>
<td>NH₃</td>
<td>Ammonia</td>
</tr>
<tr>
<td>C₂H₅N₂O₂</td>
<td>Biuret</td>
</tr>
<tr>
<td>C₃H₄N₄O₂</td>
<td>Ammeline</td>
</tr>
<tr>
<td>C₅H₅N₃O</td>
<td>Ammelide</td>
</tr>
<tr>
<td>N₂</td>
<td>Dinitrogen</td>
</tr>
<tr>
<td>NOₓ</td>
<td>Nitrogen oxide</td>
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Latin Symbols

<table>
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<tr>
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<th>Description</th>
<th>Units</th>
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<tbody>
<tr>
<td>A</td>
<td>Area</td>
<td>[m²]</td>
</tr>
<tr>
<td>b</td>
<td>Heat penetration coefficient</td>
<td>[-]</td>
</tr>
<tr>
<td>Cₚ</td>
<td>Specific heat capacity</td>
<td>[W m⁻² K⁻¹]</td>
</tr>
<tr>
<td>c</td>
<td>Local speed of sound</td>
<td>[ms⁻¹]</td>
</tr>
<tr>
<td>D</td>
<td>Diameter</td>
<td>[m]</td>
</tr>
<tr>
<td>Symbol</td>
<td>Description</td>
<td>Units</td>
</tr>
<tr>
<td>--------</td>
<td>-------------</td>
<td>-------</td>
</tr>
<tr>
<td>$e$</td>
<td>Specific internal energy</td>
<td>[J]</td>
</tr>
<tr>
<td>$E$</td>
<td>Total energy</td>
<td>[J]</td>
</tr>
<tr>
<td>$f$</td>
<td>Roughness function</td>
<td>[-]</td>
</tr>
<tr>
<td>$f_c$</td>
<td>Curvature correction factor</td>
<td>[-]</td>
</tr>
<tr>
<td>$f_2$</td>
<td>Damping function</td>
<td>[-]</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational vector</td>
<td>[$ms^{-2}$]</td>
</tr>
<tr>
<td>$H$</td>
<td>Total enthalpy</td>
<td>[J]</td>
</tr>
<tr>
<td>$k$</td>
<td>Turbulent kinetic energy</td>
<td>[J/kg]</td>
</tr>
<tr>
<td>$l$</td>
<td>Length</td>
<td>[m]</td>
</tr>
<tr>
<td>$Ma$</td>
<td>Mach number</td>
<td>[-]</td>
</tr>
<tr>
<td>$p$</td>
<td>Pressure</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$Pr$</td>
<td>Prandtl number</td>
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</tr>
<tr>
<td>$\dot{Q}$</td>
<td>Heat transfer</td>
<td>[W]</td>
</tr>
<tr>
<td>$q''$</td>
<td>Heat flux</td>
<td>[W/m²]</td>
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<tr>
<td>$Re$</td>
<td>Reynolds number</td>
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<tr>
<td>$t$</td>
<td>Time</td>
<td>[s]</td>
</tr>
<tr>
<td>$T$</td>
<td>Temperature</td>
<td>[°C] and [K]</td>
</tr>
<tr>
<td>$T^+$</td>
<td>Dimensionless temperature</td>
<td>[-]</td>
</tr>
<tr>
<td>$T_e$</td>
<td>Large-eddy time scale</td>
<td>[s]</td>
</tr>
<tr>
<td>$u$</td>
<td>Velocity</td>
<td>[ms⁻¹]</td>
</tr>
<tr>
<td>$U$</td>
<td>Velocity</td>
<td>[ms⁻¹]</td>
</tr>
<tr>
<td>$u^+$</td>
<td>Dimensionless velocity</td>
<td>[-]</td>
</tr>
<tr>
<td>$v$</td>
<td>Velocity</td>
<td>[ms⁻¹]</td>
</tr>
<tr>
<td>$y^+$</td>
<td>Dimensionless thickness</td>
<td>[-]</td>
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**Greek Symbols**

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<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Units</th>
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<tbody>
<tr>
<td>$\rho$</td>
<td>Density</td>
<td>[kgm⁻³]</td>
</tr>
<tr>
<td>$\sigma$</td>
<td>Stress</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$\lambda$</td>
<td>Thermal conductivity</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$\mu$</td>
<td>Dynamic viscosity</td>
<td>[kgm⁻¹s⁻¹]</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinetic viscosity</td>
<td>[m²/s]</td>
</tr>
<tr>
<td>$\mu_t$</td>
<td>Eddy viscosity</td>
<td>[kgm⁻¹s⁻¹]</td>
</tr>
<tr>
<td>$\delta$</td>
<td>Kronecker Delta</td>
<td>[-]</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>Dissipation of turbulence energy</td>
<td>[W/kg]</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Shear stress</td>
<td>[Pa]</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>von Karman’s constant</td>
<td>[-]</td>
</tr>
<tr>
<td>$\pi$</td>
<td>Archimedes’ constant</td>
<td>[-]</td>
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### Subscripts and superscripts

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Meaning</th>
</tr>
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<tbody>
<tr>
<td>i</td>
<td>variable index in x-direction</td>
</tr>
<tr>
<td>j</td>
<td>variable index in y-direction</td>
</tr>
<tr>
<td>w</td>
<td>wall-term</td>
</tr>
<tr>
<td>p</td>
<td>particle-term</td>
</tr>
<tr>
<td>d</td>
<td>droplet-term</td>
</tr>
<tr>
<td>f</td>
<td>running cell number</td>
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1 | Introduction

1.1 Emission standards

Since the early 90s, the European Union and the United States have introduced increasingly strict emissions standards for the vehicle industry. These emission standards define the acceptable emissions of nitrogen oxides (NO\(_X\)), carbon monoxide (CO), hydrocarbons (HC), ammonia (NH\(_3\)) and particulate matter (PM) for most vehicle types. The latest emission standard within the EU, Euro VI, deems the emission of NO\(_X\) (0.4g/kWh) and PM (0.01g/kWh) to be the most crucial components to limit for heavy-duty diesel vehicles, see table 1. This is a big difference compared to the previous EU emission legislation, Euro V, which limits of emission were NO\(_X\) 2 g/kWh and PM 0.2 g/kWh. A similar focus can be seen for the US emission legislation, as the shift from its previous emission standard to its current one display values very akin to Euro VI for the emissions of NO\(_X\) and PM (see table 1).

Table 1: Current and previous emission limits for NO\(_X\), PM, CO, HC and NH\(_3\) for heavy-duty vehicles within the European Union and the United States [1, 2].

<table>
<thead>
<tr>
<th>Region</th>
<th>NO(_X) [g/kWh]</th>
<th>PM [g/kWh]</th>
<th>CO [g/kWh]</th>
<th>HC [g/kWh]</th>
<th>NH(_3) [ppm]</th>
</tr>
</thead>
<tbody>
<tr>
<td>EU (Euro VI)</td>
<td>0.4</td>
<td>0.01</td>
<td>1.5</td>
<td>0.13</td>
<td>0.01</td>
</tr>
<tr>
<td>EU (Euro V)</td>
<td>2</td>
<td>0.2</td>
<td>1.5</td>
<td>0.46</td>
<td>-</td>
</tr>
<tr>
<td>US (current leg.)</td>
<td>0.27</td>
<td>0.013</td>
<td>20</td>
<td>0.19</td>
<td>-</td>
</tr>
<tr>
<td>US (previous leg.)</td>
<td>5.4</td>
<td>0.135</td>
<td>20</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

1.2 After-treatment for diesel engines

As a response to the ever-increasing demands on lower emissions, new technologies involving after-treatment of the exhaust from diesel engines have been adopted. A schematic of a typical current diesel engine after-treatment system is shown in figure 1. As the exhaust leaves the engine, it enters the first stage of the after-treatment system, the diesel oxidation catalyst (DOC). The task of the DOC is to oxidize the hydrocarbons, carbon monoxides and nitrogen monoxides, forming carbon dioxide and water. The next stage is a diesel particulate filter (DPF). It is made up of porous substrates, which effectively filter out and trap the soot within the exhaust.
The next stage is the urea-water evaporation system. It consists of an evaporation chamber, where a water-urea solution (UWS) is injected into the exhaust through spray. The most frequently used UWS is called AdBlue®, which consists of 32.5% urea. The purpose of the evaporation system is to produce the reducing agent ammonia ($NH_3$), which will be utilized in a selective catalytic reduction (SCR) process to minimize the amount of $NO_X$ in the exhaust. As the UWS is introduced to the system, the hot exhaust gases quickly evaporate the water of the UWS mixture, leaving the urea molten and unstable. The molten urea then undergoes thermolysis and is converted into isocyanic acid and ammonia:

$$\text{CO(NH}_2\text{)}_2 + \text{Heat} \leftrightarrow \text{HNCO} + NH_3$$

This is followed by a hydrolysis reaction, where water reacts with isocyanic acid ($HNCO$), producing carbon dioxide ($CO_2$) and further ammonia ($NH_3$):

$$\text{HNCO} + H_2O \leftrightarrow NH_3 + CO_2$$

The exhaust gases eventually enter the selective catalytic reduction (SCR) catalyst, where the produced ammonia acts as a reducing agent, converting $NO_X$ into diatomic nitrogen ($N_2$) and water ($H_2O$):

$$NO_X + NH_3 \leftrightarrow N_2 + H_2O$$

The last stage of the after-treatment system is the ammonia slip catalyst (ASC). Its task is to oxidize any remaining ammonia ($NH_3$) leaving the SCR, converting it to diatomic nitrogen ($N_2$) and water ($H_2O$).

A major problem area of this type of after-treatment system is the evaporation stage [3]. Complications can appear for both overestimating and underestimating the amount of UWS that needs to be injected for given exhaust flow conditions. As the spray hits the evaporation surface, a liquid film of UWS may take form. Given unfavourable operating conditions, there is a risk for the urea within the liquid film to crystallize and form solid deposits. These solid deposits can in turn cause high back-pressure, ammonia slip as well as threaten the structural integrity of the entire evaporation chamber [3]. Figure 2 illustrates two test cases, where growth of solid deposits have occurred as a result of UWS overdosing. Injecting too little UWS would instead lead to an amount of ammonia ($NH_3$) that is insufficient for fully reducing the $NO_X$ of the exhaust in the SCR stage.
1.3 Simulation of SCR evaporation systems

Simulation software makes it possible for R&D teams at Scania to avoid expensive physical tests at the prototype stage of development. By utilizing a simulation strategy called Design of Experiments (DOE), it becomes feasible to investigate a vast range of concepts very quickly, effectively reducing development time. New simulation methods and software are continuously being investigated and validated by simulations teams such as NXPS, to reduce development time and increase product quality.

One of the most computationally heavy processes to simulate within a silencer is the UWS spray and the subsequent prediction of solid deposit inside the evaporation system. Most CFD models used for this purpose hold a good level of accuracy and are utilized throughout the whole industry where SCR aftertreatment is applied. Despite this, these models are limited in the fact that they are only able to cover timescales in the scope of seconds to minutes while using a tolerable amount of computational power. However, the time spectrum for solid deposit formation is minutes to hours.

There exist numerous publications that focuses on the simulation of predicting the risk for solid deposit in SCR systems. Zheng evaluated a simulation tool which predicts the locations of urea deposits and validated these towards measurements. In this study it was concluded that the UWS spray and its ensuing liquid film formation, breakup and boiling need to be captured more comprehensively in order to attain an accurate description of the spray and urea behavior within the evaporation system. Smith et al developed an improved method to evaluate the deposit formation risk, that accurately predicted the risk of deposit formation and showed promising signs of speeding up the solution by focusing on the physical properties of the liquid wall film.
Another complex process to simulate accurately within a SCR evaporation system is the ammonia homogenization that takes place through a mixing process before the ammonia enters the SCR catalyst. Fischer et al. [4] has presented a study that looks into the influence that the chosen turbulence model has on the prediction of the turbulent mixing process of the gaseous ammonia. It shows that Reynolds-averaged $k-\epsilon$ models consistently underestimate the turbulence level of the swirl flow, which in turn also results in underestimation of the turbulent diffusion and uniformity of the ammonia vapour that enters the catalyst. The use of a Reynolds-Stress model instead lead to enhanced predictions, as it accounts for the anisotropic aspect of the turbulence in the swirl flow. A combination of using a Reynolds-Stress model together with detailed sub-models responsible for the liquid interphase physics resulted in a highly accurate prediction of the ammonia homogenization for a broad spectrum of operating conditions.

1.4 Scania - aftertreatment development at NXPS

Scania CV is a major Swedish manufacturer of commercial heavy-duty vehicles - specifically trucks and buses. Founded in 1891, it enjoys a rich heritage of engineering expertise within the transportation industry and currently employs over 52000 people. As a global company, Scania has become one of the leading manufacturers of heavy-duty vehicles worldwide. In its effort to produce products with lower emissions, higher performance and quiet operation, Scania continuously works to improve its after-treatment technologies. A key function to achieving this vision lies in its current line of silencers, in which the after-treatment system is fully integrated.

The UWS spray of the evaporation system is currently being simulated through AVL Fire and OpenFOAM at Scania, where AVL Fire is used as the main simulation tool for most engineers. The major drawback of using AVL Fire for spray simulations is that it is deemed too time-consuming to set up new cases, which makes it too costly in terms of expensive engineering hours. A previous master thesis project, performed by Emelie Trigell, has looked into the possibility of using STAR-CCM+ (developed by Siemens) for spray simulations at Scania [10]. One of the biggest features with STAR-CCM+ is its speedup method, which has been shown to provide a speedup for spray simulations by up to a factor of 20 [10 p.31]. STAR-CCM+ also boasts a user-friendly interface, powerful and simple mesh generation and flexible post-processing capabilities, which makes it a powerful contender to replace AVL Fire or at least take a fair share of its place as one of the main spray simulation softwares at Scania.

1.5 Thesis aim and objectives

The main aim of this project is to investigate the possibility of utilizing STAR CCM+ for simulating the UWS spray in Scania’s silencers. Part objectives of this project include:

- Performing simulations with UWS spray in STAR CCM+ to compare with
experimental data

- Evaluating how the solution is affected when changing relevant method-related parameters

1.6 Limitations

This thesis work is defined and structured within the boundaries set up in the course TQMT33, which attributes 30 ECTS credits. This corresponds to 20 working weeks, or 800 work hours.

The project was originally planned to investigate both a standard method and a speedup method for UWS spray simulations in STAR-CCM+. However, due to technical issues surrounding the compatibility of the speedup method on the Cray system at PDC, a full investigation was only possible for the standard method. Introductory theory and arguments for further investigation of the speedup method are still included. The investigation into the influence of critical parameters is still very relevant for the speedup-method.

1.7 Delimitations

In order to limit the scope of the project, delimitations are needed. The most essential delimitation for this project is that it focuses solely on computational method development and comparisons with measurements from physical testing, not on conducting new physical tests or the physical test environment.
2 | Theory

2.1 Fluid dynamics

The principles of fluid dynamics are assembled with three governing equations: the conservation of mass, conservation of momentum and conservation of energy. By implementing these three equations into a control volume, they can be discretized and utilized for doing numerical calculations on a fluid. The Reynolds number ($Re$), seen in equation (1), is a dimensionless quantity used to help predict flow characteristics such as whether a flow is laminar, turbulent or in a transition of the two.

$$Re = \frac{Inertial\ forces}{Viscous\ forces} = \frac{\rho U \ell}{\mu}$$  \hspace{1cm} (1)

where $\rho$ is the density of the fluid (kg/m$^3$), $U$ the velocity of the fluid with respect to the studied point (m/s), $\ell$ the characteristic linear dimension (m) and $\mu$ the dynamic viscosity of the fluid (kg/m·s).

When studying an ideal gas, the fluid can often be considered incompressible. However, this criteria is dependent on the Mach number ($Ma$) (see equation (2)). If $Ma \geq 0.3$, the flow must be seen as compressible.

$$Ma = \frac{u}{c}$$  \hspace{1cm} (2)

where $u$ is the velocity of the fluid (m/s) and $c$ is the local speed of sound (m/s).

Turbulence modelling

As the governing equations of fluid dynamics cannot be solved analytically except for very simple cases, numerical simulations utilizing mathematical models to simplify the calculations are used instead. Different approaches can be used in order to simulate and model the fluid flow of a system. The largest difference between most approaches is how they differ in the treatment of turbulence. Direct numerical simulations (DNS) resolve all the scales of turbulence, without resorting to any turbulence model. This however requires an extreme amount of computational power. Hence, approaches where only the largest turbulence scales are resolved, such as Large eddy simulations (LES) or similar variants, become more feasible choices. However, most of these approaches have harsh requirements on the spatial and temporal resolution, which makes simulations with high Reynolds numbers very expensive. LES approaches are also very sensitive to the initial turbulence, which is not well known inside an industrial diesel engine silencer. Thus, an URANS (unsteady Reynolds averaged numerical simulation) approach is used during the investigations of this project.
The normal RANS approach utilizes time-averaged equations of motion to describe the fluid flow. First the instantaneous variables are decomposed into its time-averaged and fluctuating quantities:

\[ v = \bar{v} + v' \]  

where \( \bar{v} \) denotes the time-averaged component and \( v' \) denotes the fluctuating component.

In the incompressible form, the RANS equations are read as [11, p.185]:

\[ \frac{\partial \bar{u}_i}{\partial x_i} = 0 \]  
\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} (\bar{u}_i \bar{u}_j) = - \frac{1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial u'_i u'_j}{\partial x_j} \]  

The URANS equations consists of the normal RANS equations, but with the transient (unsteady) term included. The dependent variables are now thus function of time, i.e. \( \bar{u}_i = \bar{u}_i(x_1, x_2, x_3, t), \ p = \bar{p}(x_1, x_2, x_3, t) \) and \( \bar{u}'_i u'_j = u'_i u'_j(x_1, x_2, x_3, t) \).

Although the results from a URANS simulation are unsteady, the time-averaged flow is still the main subject of interest. The time-averaged component is denoted as \( \langle \bar{v} \rangle \), which implies that the results of the URANS can be decomposed as a time-averaged part, \( \langle \bar{v} \rangle \), a resolved fluctuation, \( v' \) and a modelled, turbulent fluctuation, \( v'' \). Thus equation (6) is attained:

\[ v = \bar{v} + v'' = \langle \bar{v} \rangle + v' + v'' \]  

For compressible flows, density changes with the pressure, and thus these variations enter the averaged form of the governing equations. A technique called Favre averaging can be used to avoid introducing these additional terms into the governing equations. The Favre-average of a variable, \( \bar{v} \), is defined as:

\[ \tilde{v} = \frac{\bar{v}}{\bar{p}} \]  

where the overline denotes the Reynolds averaged value.

The instantaneous value of the Favre-average is decomposed by:

\[ v = \tilde{v} + v'' \]  

where the \( v'' \) denotes the fluctuating part with regards to the Favre averaging.
Utilizing equations (7) and (8), the Favre-averaged form of the three governing equations can be arranged [12]:

Conservation of mass

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i} (\rho \tilde{u}_i) = 0 \tag{9}$$

Conservation of momentum

$$\frac{\partial}{\partial t} (\rho \tilde{u}_i) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_i \tilde{u}_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} (\tau_{ij} - \rho u''_i u''_j) \tag{10}$$

Conservation of energy

$$\frac{\partial}{\partial t} (\rho E) + \frac{\partial}{\partial x_j} (\rho \tilde{u}_j H) = \frac{\partial}{\partial x_j} (\tilde{u}_i \tau_{ij} - \tilde{u}_i \rho u''_i u''_j) + \frac{\partial}{\partial x_j} \left[ -q_{ij} - q_{ij} + \tau_{ij} u'_i - \rho u''_j u''_i \right] \tag{11}$$

where \( E = \tilde{\varepsilon} + \frac{1}{2} \tilde{u}_i \tilde{u}_i + k \) is the total energy and \( H = \tilde{\varepsilon} + \frac{\tilde{p}}{\tilde{\rho}} + \frac{1}{2} \tilde{u}_i \tilde{u}_i + k \) the total enthalpy, in which \( \tilde{\varepsilon} \) is the Favre-averaged form of the internal energy, \( \varepsilon \).

\[ k = \frac{1}{2} \frac{\rho u''_i u''_j}{\tilde{\rho}} \] is the turbulent kinetic energy, \( q_{ij} = -\frac{C_p \mu}{P_{rl}} \frac{\partial \tilde{T}}{\partial x_j} \) is the heat-flux vector, where \( P_{rl} = \frac{C_p \mu}{\lambda} \) is the molecular Prandtl number in which \( C_p \) is the specific heat, \( \lambda \) the thermal conductivity and \( \mu \) the dynamic viscosity. \( q_{ij} = -\frac{\mu \tilde{\rho} u''_i u''_j}{P_{rl} \tilde{\rho}_x} \) is the molecular heat-flux vector, in which \( \mu_{t} \) is the eddy viscosity (see equation (13)), \( P_{rl} = \frac{\epsilon^M}{\epsilon^H} \) is the turbulent Prandtl number, with \( \epsilon^M \) as the eddy diffusivity for momentum transfer and \( \epsilon^H \) as the eddy diffusivity for heat transfer.

The averaging of the governing equations has introduced a new property, the Reynolds stresses, \( \tau \). The Reynolds stresses are unknown stresses caused by the turbulence and their existence poses the dilemma of having more variables than equations, often referred to as the "closure problem". A common way to solve the closure problem was developed by Joseph Valentin Boussinesq. Boussinesq postulated that, just as the viscous stresses are proportional to the mean rate of deformation of the flow for Newtonian fluids, the turbulent Reynolds stresses can be related to the mean rate of deformation of the flow by introducing the variable "eddy viscosity" [13] p.29:

$$\tau_{ij} = -\rho u''_i u''_j = \mu_t \left( \frac{\partial U_i}{\partial x_j} + \frac{\partial U_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_i} \delta_{ij} \right) - \frac{2}{3} \rho k \delta_{ij} \tag{12}$$
where \( \mu_t \) is the eddy viscosity, calculated as:

\[
\mu_t = \rho C_{\mu} f_{\mu} k T_e
\]

(13)

in which \( \rho \) is the density, \( C_{\mu} \) a model coefficient, \( f_{\mu} \) a damping function, \( T_e = \frac{k}{\epsilon} \) the large-eddy time scale and \( \delta_{ij} \) is the Kronecker’s delta.

Turbulence models that utilize the relation in equation (12) are called eddy-viscosity models. The model that is supported by the spray methods in STAR-CCM+ is the realizable \( k-\epsilon \) two-layer turbulence model [14]. It solves two transport equations: that of the turbulent kinetic energy (\( k \)):

\[
\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho k \mathbf{v}) = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right] + P_k - \rho (\epsilon - \epsilon_0) + S_k
\]

(14)

and the rate of dissipation of turbulence energy (\( \epsilon \)).

\[
\frac{\partial}{\partial t} (\rho \epsilon) + \nabla \cdot (\rho \epsilon \mathbf{v}) = \nabla \cdot \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right] + \frac{1}{T_e} C_{\epsilon 1} P_\epsilon - C_{\epsilon 2} f_2 \rho \left( \frac{\epsilon}{T_e} - \frac{\epsilon_0}{T_0} \right) + S_\epsilon
\]

(15)

where \( \mathbf{v} \) is the mean velocity, \( \mu \) the dynamic viscosity, \( P_k \) and \( P_\epsilon \) are production terms, \( \sigma_k \), \( \sigma_\epsilon \), \( C_{\epsilon 1} \), \( C_{\epsilon 2} \) and \( C_\ell \) are model coefficients, \( f_2 \) a damping function, and \( S_k \) and \( S_\epsilon \) are user-specified source terms. \( \epsilon_0 \) is the ambient turbulence value in the source terms with a specific time scale: \( T_0 = \max \left( \frac{k_0}{\epsilon_0}, C_\ell \sqrt{\frac{T}{\epsilon_0}} \right) \), in which \( \nu \) is the kinematic viscosity and \( C_\ell \) a model coefficient. See appendix A.1 for a full explanation of all the terms in the equations.

**Near-wall treatment**

Walls are a source of vorticity for most flow problems. Being able to accurately predict the flow across a wall is thus very important. In fluid mechanics, the thin viscosity-influenced layer of the flow region innermost to a wall can be split into three distinct subregions (see figure 3): the viscous sublayer, the buffer layer and the log-law layer. The thickness of these different layers is prescribed by the non-dimensional wall distance, \( y^+ \), see equation (16). Similarly, the non-dimensional velocity \( u^+ \) and temperature \( T^+ \) are defined through equation (17) and (18) respectively. [15] p.57

\[
y^+ = \frac{y}{l_*} = \frac{yu_\tau}{\nu}
\]

(16)

\[
u^+ = \frac{U}{u_\tau}
\]

(17)

\[
T^+ = \rho C_p u_\tau \frac{T - T_w}{q''}
\]

(18)
where $\nu$ is the kinematic viscosity, $u_\tau$ the friction velocity $u_\tau = \sqrt{\frac{\tau_w}{\rho}}$, $l_*$ the viscous length scale $l_* = \frac{\nu}{\mu_\tau}$, $y$ the dimensional distance from the wall, $U$ the dimensional velocity, $\rho$ the density, $C_p$ the specific heat, $T$ the temperature, $T_w$ the temperature of the wall and $q''$ the wall heat flux (see equation (30) in the chapter Conjugate heat transfer of section 2.2).
Integrating with respect to $y$ and applying the boundary condition $U(y = 0) = 0$, the following relationship between the mean velocity and the distance from the wall can be made \[15\] p.58:

$$U = \frac{\tau_w y}{\mu}$$ (20)

Applying the definitions of $y^+$ and $u^+$ results in equation \[21\], which displays a linear relationship between the two dimensionless parameters \[16\] \[15\] p.58:

$$u^+ = y^+$$ (21)

Furthermore, the dimensionless temperature $T^+$ can be related to the dimensionless thickness $y^+$ as seen in equation \[22\]:

$$T^+ = Pr y^+$$ (22)

where $Pr = \frac{C_p \mu}{\lambda}$ is the Prandtl number, with $C_p$ as the specific heat, $\mu$ the dynamic viscosity and $\lambda$ the thermal conductivity.

**Log-law layer**

The log-law layer is the turbulent region close to a smooth wall. Where it exists ($30 < y^+ < 500$), the inertial forces dominate the viscous. Within this region, the relationship between $u^+$ and $y^+$ takes on a logarithmic form, as seen in equation \[23\] \[15\] p.58:

$$u^+ = \frac{1}{\kappa} \ln(y^+) + B = \frac{1}{\kappa} \ln(Ey^+)$$ (23)

where $\kappa = 0.4$ is the von Karman’s constant, $B \approx 5.5$ and $E \approx 9.8$ for smooth walls.

Additionally, the relationship between the dimensionless temperature $T^+$ and the dimensionless thickness $y^+$ also take on a logarithmic form, see equation \[24\]:

$$T^+ = Pr_t \left[ \frac{1}{\kappa} \ln(E' y^+) + P \right]$$ (24)

where $Pr_t = \frac{\epsilon_M}{\epsilon_H}$ is the turbulent Prandtl number, with $\epsilon_M$ as the eddy diffusivity for momentum transfer and $\epsilon_H$ as the eddy diffusivity for heat transfer. See appendix A.2 for a full explanation of all the terms in the equations.
**Buffer layer**

The buffer layer (5 < \( y^+ < 30 \)) is the transition stage between the laminar, viscous sub-layer and the turbulent log-law sub-layer. Within it, neither the linear relation of the viscous boundary layer or the log-law of the log-law layer holds. It is difficult to model accurately and thus it is advisable to keep the first cell either within the viscous sub-layer or the log-law layer.

**Hybrid wall treatment**

For the studied methods in STAR-CCM+, the liquid film model demands that the first cell layer centroid should always be twice that of the liquid film thickness (see **Liquid film** chapter in section 2.2). Thus placing the first cell within the log-law region might seem advisable. However, to properly resolve the heat transfer at the wall, the first cell layer centroid should be placed within the viscous sub-layer \[16\]. For high Reynold’s flows such as the ones studied in this project, the flow velocity remains high. Furthermore, the transient nature of the spray injections and the potentially growing liquid film of the evaporation surfaces also impose larger fluctuations of the actual values of the non-dimensional parameters \( y^+ \), \( u^+ \) and \( T^+ \). Thus, the first cell layer centroid could potentially be located within the buffer layer or even the log-law region as a result (unless an extremely fine mesh is used). This issue is reasonably solved through the two-layer all-\( y^+ \) wall treatment. This hybrid wall treatment uses blending functions to calculate the value of \( u^+ \) and \( T^+ \) (see equation (25) and (26)). These blending functions are formulated with the desirable characteristic of producing reasonable answers even for the case when the first cell layer centroid falls within the buffer layer.

In the two-layer all-\( y^+ \) wall treatment, the blended wall function for the relationship between the dimensionless velocity \( u^+ \) and the dimensionless thickness \( y^+ \) is defined according to Reichhardt’s law \[17\]:

\[
\begin{align*}
  u^+ &= \frac{1}{\kappa} \ln (1 + \kappa y^+) + C \left( 1 - e^{y^+/y_m^+} - \frac{y^+}{y_m^+} e^{-by^+} \right) \\
  C &= \frac{1}{\kappa} \ln \left( \frac{E'}{\kappa} \right), \quad b = \frac{1}{2} \left( \frac{y_m^+ \kappa}{C} + \frac{1}{y_m^+} \right), \\
  y_m^+ &= \max \left[ 3, 267(2.64 - 3.9\kappa)E'^{0.0125} \right] - 0.987
\end{align*}
\] (25)

The blended wall function for the relationship between the dimensionless temperature \( T^+ \) and the dimensionless thickness \( y^+ \) is defined according to Kader’s law \[18\]:

\[
\begin{align*}
  T^+ &= \exp \left( -\Gamma \right) Pr_y y^+ + \exp \left( -\frac{1}{\Gamma} \right) Pr_t \left[ \frac{1}{\kappa} \ln (E'y^+) + P \right]
\end{align*}
\] (26)
where
\[ \Gamma = \frac{0.01 c (Pr y^+)^4}{1 + \frac{5}{c} Pr^3 y^+}, \quad c = \exp(f - 1) \]

in which \( f \) is a roughness function. See appendix A.2 for a full explanation of all the terms in the equations.

### 2.2 Modelling the UWS spray process

The modelling of UWS spray is done through a Lagrangian framework consisting of a dispersed phase of UWS droplets. Since the number of droplets can become very high and thus heavily impact the computational time, a smaller number of computational parcels instead represent the total population of droplets. Within this section, any model or equation that is not referenced externally has either been designed by Siemens or been adopted without reference into the spray simulation methods of STAR-CCM+.

**Urea Evaporation**

Evaporation of urea is modelled through the *Quasi Steady Evaporation model*. This model allows droplets to lose mass through evaporation. The driving force for evaporation is the departure from equilibrium of the liquid-vapor system, shown as an idealized phase diagram in figure 4. There are two material properties that decide the vaporization line: the saturation pressure and the critical temperature.

![Figure 4: Idealized vaporization system used in the Quasi Steady Droplet Evaporation model. Beyond the critical point, the rate of evaporation increases rapidly and vapour becomes the dominating phase regardless of the pressure.](image-url)
Droplet-Wall interaction

The outcome of when a liquid droplet impinges on a wall is determined by the Bai-Gosman Wall Impingement model [19]. There are six possible outcomes, see figure 5.

Figure 5: Droplet Outcomes for the Bai-Gosman Wall Impingement model. Adhere = droplets stick to the surface, Rebound = droplets bounce on the evaporation surface and continue being tracked, Spread = droplets break and form liquid film, Break-up and rebound = droplets break-up into smaller droplets and rebound as they hit the evaporation surface, Break-up and spread = droplets break-up into smaller droplets and spread across the evaporation surface, Splash = droplets breaks up into smaller droplets, some of which are reflected from the evaporation surface.

Four parameters are evaluated to choose the outcome:

1. The Weber number, \( W_{cl} = \frac{\rho_p v_{r,n}^2 D_p}{\sigma} \)

2. The Laplace number, \( La = \frac{\rho_p \sigma D_p}{\mu_p^2} \)

3. The wall temperature, \( T_w \)

4. Whether the wall is wet or dry

where \( \rho_p \) is the density of a particle, \( v_{r,n} \) the relative velocity of a particle with regards to the wall that is impinged, \( D_p \) the diameter of a particle, \( \mu_p \) the dynamic viscosity of a particle and \( \sigma \) the surface tension.
Figures 6 and 7 illustrate the impingement modes for different ranges of temperature and Weber numbers for a dry and wet wall, respectively.

<table>
<thead>
<tr>
<th>We</th>
<th>Temperature Range 1</th>
<th>Temperature Range 2</th>
<th>Temperature Range 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>We&lt;sub&gt;0&lt;/sub&gt;</td>
<td>Splash</td>
<td>Splash</td>
<td>Splash</td>
</tr>
<tr>
<td>We&lt;sub&gt;12&lt;/sub&gt;</td>
<td>Spread</td>
<td>Breakup and Spread</td>
<td>Spread</td>
</tr>
<tr>
<td>We&lt;sub&gt;25&lt;/sub&gt;</td>
<td>Rebound</td>
<td>Spread</td>
<td></td>
</tr>
</tbody>
</table>

Figure 6: Impingement modes for a dry wall. \( T_{12} \) is expected to be approximately the boiling temperature of the droplet. \( T_{23} \) is expected to be approximately the lower transition temperature\(^1\) of the droplet.

<table>
<thead>
<tr>
<th>We</th>
<th>Temperature Range 1</th>
<th>Temperature Range 2</th>
<th>Temperature Range 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>We&lt;sub&gt;0&lt;/sub&gt;</td>
<td>Splash</td>
<td>Splash</td>
<td>Splash</td>
</tr>
<tr>
<td>We&lt;sub&gt;12&lt;/sub&gt;</td>
<td>Breakup and Spread</td>
<td>Breakup and Spread</td>
<td></td>
</tr>
<tr>
<td>We&lt;sub&gt;25&lt;/sub&gt;</td>
<td>Rebound</td>
<td>Rebound</td>
<td>Spread</td>
</tr>
</tbody>
</table>

Figure 7: Impingement modes for a wet wall. \( T_{12} \) is expected to be approximately the boiling temperature of the droplet. \( T_{23} \) is expected to be approximately the lower transition temperature of the droplet.

\(^1\)See Liquid film chapter
The heat transfer that takes place during wall impingement is modelled through the *Impingement heat transfer model*. The transferred heat from wall to droplet is calculated by the Wruck correlation \[20\]:

\[
\dot{Q}_{w-d} = A_{cont} \frac{2\sqrt{t_{cont}}}{\sqrt{\pi}} \frac{b_w b_d}{b_w + b_d} (T_w - T_d)
\]  

(27)

where \(w\) and \(d\) refer to terms of the wall and droplet, respectively, \(A_{cont}\) is the effective contact area: \(A_{cont} = \pi D_{eff}^2\), \(t_{cont}\) is the contact time between droplet and wall and \(b\) is the heat penetration coefficient as evaluated with the materials of the wall or droplet.

**Liquid film**

The injected UWS takes time to evaporate and is thus sprayed onto an evaporation surface, to promote liquid film formation and subsequent evaporation. The *Fluid Film model* is used to capture this physics. Assumptions that are made in the fluid film model formulation include:

- A parabolic velocity profile through the film
- The film is thin enough to treat the boundary layer as laminar
- The film stays attached to the boundary
- The analysis is transient, as the SCR process is highly unsteady

The heat transfer between the wall and the liquid film can be seen as a function of surface excess temperature according to the Nukiyama-pool boiling model \[21\] p.496, see figure [8].
I) Below the saturation temperature (boiling point), $T_{sat}$, the dominating source of heat transfer is natural convection.

II) In the near wall region, vapor bubbles are formed, which help support the heat transport within the liquid.

III) As the excess temperature increases, the vapor bubbles start to merge into slugs and columns, which further supports the heat transfer, until a maximum value of heat flux (critical heat flux) is reached, at $T_{Nukiyama}$. This is the point where the liquid wetting of the wall is at its peak.

IV) At even higher temperatures, the local boiling spots start to break up, forming a growing vapor film at the fluid-solid interface (transition boiling). This reduces the heat transfer down to a local minimum at $T_L$ (Leidenfrost temperature), whereupon a continuous insulating vapor cushion has been formed between the wall and liquid (Leidenfrost phenomenon [5, 22]). The vapor cushion also dramatically reduces the adhesion of the droplets to the wall.

V) For temperatures beyond $T_L$, thermal radiation through the vapor cushion is the dominating source of heat flux (film boiling).

As a vapor cushion effectively eliminates adhesion, the Leidenfrost temperature as defined by the Nukiyama curve could be used as a criterion to distinguish between wall-wetting and non-wetting regimes for liquid attached to the wall. However, the behavior of the liquid is highly unstable within the transition boiling stage (see stage four in figure 8), ranging from massive wall wetting at the Nukiyama...
temperature to absolutely no wall wetting at the Leidenfrost temperature. These constantly changing conditions are hard for a model to accurately capture, and as such a simplified wall wetting transition temperature (called the "Lower transition temperature") is used instead. It is estimated to be:

\[
T_{\text{lower transition}} = 207 + T_{\text{sat}}
\]  

(28)

**Conjugate heat transfer**

Correctly predicting the temperature of the metal spray evaporation surfaces is of high importance when it comes to predicting the liquid film formation and its consequent evaporation. It is thus essential to include the spray evaporation surfaces as solid components. The result of excluding the solid components would lead to under-prediction of the spray surfaces temperatures (which in turn leads to over-prediction of film formation and under-prediction of film evaporation).

Solids have thermal inertia. This has the fallout that equilibrium temperatures for the metal spray evaporation surfaces might not be reached for a long time (≈100s). A liquid film develops slowly and increases the real simulation time.

The heat transfer between the solid-film interface is governed by the following equation:

\[
\frac{d}{dt} \int_V \rho C_p T dV = -\oint_A q' \cdot da + \int_V sdV
\]  

(29)

where \( \rho \) is the density, \( C_p \) the specific heat, \( T \) the temperature and \( q' \) the heat flux across the solid-film interface, see equation (30)

\[
q' = \frac{T_{w-\text{solid}} - T_{w-\text{film}}}{R}
\]  

(30)

where \( T_{w-\text{solid}} \) and \( T_{w-\text{film}} \) are the interface temperatures on the solid side and liquid film side respectively and \( R \) is the thermal resistance of the interface.

The first term in the left hand side of equation (29) is the transient term. For a steady state solution, the actual value of \( \rho C_p \) does not matter, and thus the value of \( \rho C_p \) can be adjusted in order to hasten the temperature development of the film.

This way of hastening the film temperature is introduced in STAR-CCM+ as the scaling factor (SF). The heat transfer between the impinging particles and the wall is scaled through the heat penetration coefficient (HPC multiplier), which is equal to \( \sqrt{SF} \). The time scales approximately linearly with the scaling factor, and should thus be multiplied with it when assessing the results, i.e. a simulation spanning 10 seconds would with a scaling factor of 10 give temperature data for 100 seconds. The liquid film thickness does not scale in the same manner as the liquid film temperature, and should thus be evaluated with the actual simulated time instead of the scaled one [23].
2.3 UWS spray simulation methods in STAR-CCM+

**Standard method.** The standard method for simulating UWS spray in STAR CCM+ is the main focus of investigation in this project. It is set up by defining a physics continuum, liquid film, Lagrangian multi-phase (AdBlue® spray) and the interactions of the multi-phase. Below follows a list of all the models used in the standard method:

- **Physics continuum:** unsteady, three-dimensional, ideal gas (compressible), multi-component gas (air, ammonia and water), non-reacting, realizable k-epsilon two layer turbulence model, gravity, segregated flow and fluid temperature with a two-layer all y+ wall treatment.
- **Liquid film:** multi-component liquid (water and isocyanic acid), Bai-Gosman wall impingement, droplet evaporation, impingement heat transfer, turbulent dispersion and two-way coupling
- **Lagrangian multi-phase (the AdBlue® spray):** multi-component liquid (water and isocyanic acid) with two-way coupling
- **Multi-phase interactions:** impingement, film evaporation/boiling, droplet evaporation

This method utilizes a lumped approach for the evaporation and decomposition of UWS. The actual chemical inter-phase reactions of the liquid film are thus not modelled and hydrodynamic risk factors are used for assessing the formation risk of solid deposits instead. The risk criteria used for solid deposit formation can be found in section 2.4.

Since the physical characteristics of the dispersed phase in the spray are tremendously different than those of the liquid film, the two physics inhibit vastly different requirements for the time step. The AdBlue® spray is injected in short bursts and is thus only simulated during short periods. The time-step has to remain very low during injection in order to accurately capture the physics of all the multi-phase parcels injected into the Lagrangian space. Re-simulating the spray every spray period makes up the majority of the computational time, even for cases where the spray injection is very short.

**Speedup method.** The speedup method developed by Siemens relies on a co-simulation of the computationally heavy AdBlue® spray (Lagrangian multiphase) and the liquid film.

The method always starts off by running one spray period with actual simulation of the AdBlue® spray. Throughout this spray period, the source terms for momentum and energy of the gas and UWS droplets are continuously recorded and saved. These source terms are then utilized as boundary conditions for the liquid film simulation. The liquid film simulation can then run several spray periods with a larger timestep and without having to simulate the complex physics of the Lagrangian multiphase.
every spray period. This coupled way of simulating both physics enables simulations to span longer in physical time, without compromising accuracy or computational time.

As stated in figure 6 and 7, the wall temperature and Weber number are the main deciding factors for the outcome of when a droplet impinges on a wall. The temperature of the evaporation surfaces will change during the liquid film simulation. As long as the temperature remains above or below the lower transition temperature, the outcome of impingement will stay the same. However if the lower transition temperature is crossed, the boundary conditions for the outcome of impingement will change drastically. Therefore, if a set percentage of the spray evaporation surface has experienced this crossover in temperature, the spray simulation has to be rerun in order to maintain accuracy.

2.4 Determining deposit risk

In order to model the formation of solid deposits within the liquid film, inter-phase reactions have to be simulated. For urea, the numerous reactions that form deposits make up a complex network of reactions (see figure 9) that unfortunately the inter-phase modelling in STAR-CCM+ cannot capture. To predict the formation of solid deposits, a probability assessment including the hydrodynamic and chemical risks can be used instead.

Figure 9: Reaction network for urea decomposition with byproduct formation and decomposition. Reprinted from A. M Bernhard [24, p.97], Copyright (2018) with permission from Elsevier.
Hydrodynamic risk factors The initial footprint of the liquid film and its subsequent pathway as well as the liquid film thickness, velocity and dynamics can all be utilized for assessing the risk of solid deposit formation. The pathway of the liquid film display areas where it is possible for deposits to accumulate [25, p.536]. Areas with high liquid film thickness depend on the dynamics of the film for accurate risk assessment. High dynamics indicate transport areas of film and thus the risk for solid deposit is low, whereas high liquid film thickness areas with low dynamics are considered to be deposit risk areas [25, p.537]. The initial footprint of the liquid film is generally not a risk area, as the dynamics of the continuously growing film are too fierce for the formation of solid deposits to happen [25, p.536]. The wall film dynamics (WFD) can be analysed through the WFD-equation [25, p.536], which describes how the liquid film mass fluctuates for a specific period near the end of the simulated period:

$$WFD = \frac{\Delta m_{max}}{m_0} = \frac{m_{max} - m_{min}}{m_0},$$

where for each cell face exposed to wall wetting, $m_{max}$ and $m_{min}$ are the maximum and minimum liquid film masses throughout the specified period and $m_0$ the initial liquid film mass at the beginning of the specified period. For areas where the wall film dynamics reach above a specified threshold $WFD \geq WFD_c$, there is no risk for deposit [25, p.536].

Figure 10: Temperature regimes for the decomposition and crystallisation of urea. At temperatures below 133°C, should the concentration of urea be sufficient, there is a risk for it to crystallize. Between 133°C and 160°C, there is no solid deposit risk. Above 160°C, the decomposition of urea starts to increase significantly, which may result in the formation of solid deposits such as biuret and cyanuric acid, which do not decompose until around 350°C. As the temperature advances beyond 250°C, ammelide and ammeline may start to form as solid deposits. These substances do not decompose until 700°C, which transcends the operating temperature of a diesel engine.

Chemical risk factors Although the inter-phase modelling in STAR-CCM+ does not compute any chemical reactions, the chemical risk factors are still of use when assessing the risk for solid deposit for spray simulations in STAR-CCM+. This is
because the liquid film temperature is the main deciding factor for activating the relevant chemical reactions that can form deposits. As depicted in figure 10, for liquid film temperatures below 133°C, there is a risk for the urea to recrystallize if the concentration of urea is sufficient. At temperatures above 133°C, the urea starts to slowly decompose into ammonia (NH₃) and isocyanic acid (HNCO). Since the loss of urea is so low there is no risk for deposit formation. The decomposition of urea remains slow until 160°C, where it starts to increase significantly and secondary reactions become more frequent. These secondary reactions produce by-products such as biuret (C₂H₅N₃O₂), which formation can be sufficient for forming solid deposits if the concentration of gaseous HNCO is above a threshold value. At even higher temperatures, high concentrations of HNCO can result in the formation of ammelide (C₃H₄N₄O₂) and ammeline (C₃H₅N₅O). These two solid deposits decompose at temperatures above 700°C, well beyond the operating temperature of a diesel engine.
3 | Method

Computational resources for most heavy simulations were provided by the high performance computing center PDC, courtesy of KTH Royal Institute of Technology. PDC is the leading provider of high performance computing services for academic research in Sweden. Its main system Beskow, sports a Cray XC40 with a peak performance of nearly 2.5 Petaflops.

The software used for CFD simulations is STAR CCM+. Tools for post-processing includes STAR CCM+ as well as Matlab. This report is written in Latex (via Overleaf).

3.1 Akvariet - test rig

Carrying out simulations of a full silencer case is a very computationally demanding task. Hence, a simple geometry of a smaller Scania test rig, Akvariet (see figure 11), has been used for the initial investigations of the influence of critical parameters on the solution. It consists of an inlet, a 3 mm thick spray evaporation plate of stainless steel, windows for deposit detection during testing and an outlet. The spray injector nozzle is placed at the top, angled 30° to the normal of the spray evaporation plate.

3.1.1 Measurement data

In order to study the sensitivity of the Standard method for different flow conditions within the Akvariet test rig, three flow cases where the inlet temperature, mass
flow and UWS dosing are varied have been considered for simulations, see table 2. Experimental tests for all of these flow cases have been carried out by Constantin Nottbeck for the Akvariet test rig during a previous master thesis project at Scania [26].

Table 2: Data setup for the investigated cases of Akvariet. Temperature is the temperature of the flow at the inlet, dosing is the amount of AdBlue® being injected per minute through the injector. Deposit outcomes: *Pool = High amount of liquid film spread throughout the spray evaporation plate, Deposit = solid deposits appearing along the plate. **Approximate Reynolds number at the start of the evaporation chamber, where the spray is injected.

<table>
<thead>
<tr>
<th>Case</th>
<th>Temperature [°C]</th>
<th>Mass flow [kg/h]</th>
<th>Dosing [g/min]</th>
<th>Reynolds number** [-]</th>
<th>Deposit outcome in testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>180</td>
<td>400</td>
<td>5</td>
<td>5.7 \cdot 10^4</td>
<td>Pool*</td>
</tr>
<tr>
<td>B</td>
<td>242</td>
<td>400</td>
<td>5</td>
<td>5.2 \cdot 10^4</td>
<td>Deposit</td>
</tr>
<tr>
<td>C</td>
<td>275</td>
<td>850</td>
<td>10</td>
<td>1.06 \cdot 10^5</td>
<td>None</td>
</tr>
</tbody>
</table>

The temperature along the spray evaporation plate was recorded with seven different temperature probes during testing, see figure [12].

![Figure 12: A display of the temperature probes used during testing for the Akvariet test rig.](image)

**3.1.2 Computational domain**

For the Akvariet geometry, a base cell size of 4.0 mm was used. The surface refinement of the spray evaporation plate was set to 1.5 mm and the volume refinement at the injection region was set to 0.5 mm (see figure [13]). The cell growth rate was set to 1.3, allowing for a smooth transition between the near wall region and the bulk flow. The first prism layer was set up so that the liquid film thickness would never exceed half of its thickness. In order to resolve the temperature gradients of the solid spray evaporation plate, it was meshed in three layers using the thin mesher function, as recommended by Siemens.
3.1.3 Investigation of critical parameters

RANS-simulations of the flow were performed for all three data setups to obtain an initial condition of the flow before any transient spray simulations were run.

Mesh study The mesh is built up by polyhedral cells. Polyhedral cells contain more connections to other cells than hexagonal cells, which enables higher quality meshes for complex geometries. A mesh independency study for the Akvariet geometry was performed by Emelie Trigell during a previous master thesis project at Scania [10]. It recommends using a base size of 4.0 mm along with a surface refinement of 1.5 mm for the spray evaporation plate [10, p. 29]. This project aims to add to that study by investigating whether a refinement of the spray injector region (see figure 13) would provide any better accuracy of the solution. The investigated range of volume refinements for the injector region include: 4.0 mm, 2.0 mm, 1.0 mm and 0.5 mm. Only the volume refinement at the injector region is changed, all other mesh-related parameters are constant. Data setup used for all simulations is case A, simulated physical time is one second.

Parcel streams study Using a sufficient number of parcel streams is essential for accurately representing the droplet size distribution of the spray. Without an accurate distribution, the resulting build-up of liquid film along the spray evaporation plate might be very different from reality. From Trigell’s findings, parcel stream numbers of 50 and 100 yielded an apparent striped pattern when observing the liquid film thickness. Increasing the number of parcel streams to 200 eliminated the numerical artefact and the liquid film thickness became more evenly distributed [10, p. 27]. From these findings, it is possible that further increments to the number of parcel streams might have an effect on the solution. Hence, three different numbers of parcel streams were selected for investigation, 200, 360 and 520. Data setup for all simulations is case A, simulated physical time is one second.

Frozen flow study As the investigations of the speedup-method for spray simulations in STAR-CCM+ came to a halt (see section 1.6), interest into how to speed up the standard method started to grow instead. One way to speed up the standard method is by freezing the momentum equations of the flow when possible and reducing the number of inner iterations while the flow is frozen. The inner iterations is the number of times the solver calculates the solution for every time step,
in order to achieve convergence. Freezing the momentum equations would yield a smaller difference in the solution from one time step to the next, and thus the inner iterations needed to reach convergence for each time step should become lower. See Table 3 for the investigated cases.

Freezing the flow should only be done when the flow is considered to be in a steady state. Thus, the flow can only be frozen during constant spray and while there is no spray. The injector has a small ramp when being turned on and off, and any injected parcels need to have travelled to the point of depletion before the flow can be considered steady state.

Table 3: The three different cases investigated for the frozen flow study. Data setup for all simulations is case A, simulated physical time is ten seconds.

<table>
<thead>
<tr>
<th>Case</th>
<th>Momentum equations frozen during steady state</th>
<th>Inner iterations</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>No</td>
<td>10</td>
</tr>
<tr>
<td>Frozen - CII (constant inner iterations)</td>
<td>Yes</td>
<td>10</td>
</tr>
<tr>
<td>Frozen - VII (variable inner iterations)</td>
<td>Yes</td>
<td>3 (while momentum equations are frozen), 10 (while momentum equations are active)</td>
</tr>
</tbody>
</table>

3.1.4 Comparison with experiments

After the initial investigations of critical parameters had been completed for the Akvariet geometry, the resulting recommended settings (see section 5.1.1) were used for simulations running for an extended amount of time, with the purpose of being able to compare the simulation results with experimental results.
### 3.2 Large Silencer

Simulations have also been carried out for a real full-scale Scania silencer, the Large Silencer (see figure 14). This silencer uses an aftertreatment system composed of an inlet pipe, DOC (diesel oxidation catalyst), DPF (diesel particulate filter), evaporation system, SCR (selective catalytic reduction), ASC (ammonia slip catalyst) and an outlet pipe.

![Diagram of Large Silencer](image)

**Figure 14**: Geometry of the Scania Large Silencer. It consists of an inlet pipe, DOC (diesel oxidation catalyst), DPF (diesel particulate filter), evaporation system, SCR (selective catalytic reduction), ASC (ammonia slip catalyst) and an outlet pipe.

#### 3.2.1 Computational domain

The main focus area of this project is the evaporation chamber. In order to reduce the number of cells and thus the computational time of the simulations, the full geometry of the Large Silencer was only used for the initial RANS-simulations of the flow. For the spray simulations, only a part of the complete geometry was used for the computational domain. The included part has its inlet at the start of the DPF and its outlet at the end of the SCR, see figure 15.
For the Large Silencer, a base cell size of 5.0 mm was used. The surface refinement of the spray evaporation surface was set to 1.5 mm and the volume refinement at the injection area was set to 0.5 mm. The cell growth rate was set to 1.3, allowing for a smooth transition between the near wall region and the bulk flow. The first prism layer was set up so that the liquid film thickness would never exceed half of its thickness. In order to resolve the temperature gradients of the solid spray evaporation plate, it was meshed in three layers using the thin mesher function, as recommended by Siemens.

### 3.2.2 Measurement data

Experimental tests for the Large Silencer were carried out throughout the project. In order to study the sensitivity of the Standard method for different flow conditions within the Large Silencer, three flow cases where the inlet temperature, mass flow and UWS dosing are varied have been considered for simulations, see table 4.

**Approximate Reynolds number at the start of the evaporation chamber, where the spray is injected.**

<table>
<thead>
<tr>
<th>Case</th>
<th>Temperature [°C]</th>
<th>Mass flow [kg/h]</th>
<th>Dosing relative to case F</th>
<th>Reynolds number** [-]</th>
<th>Deposit outcome in testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>230</td>
<td>450</td>
<td>0.13</td>
<td>4.0 · 10⁴ (turb.)</td>
<td>Deposit</td>
</tr>
<tr>
<td>E</td>
<td>350</td>
<td>1500</td>
<td>0.94</td>
<td>1.14 · 10⁵ (turb.)</td>
<td>None</td>
</tr>
<tr>
<td>F</td>
<td>350</td>
<td>1500</td>
<td>1</td>
<td>1.14 · 10⁵ (turb.)</td>
<td>Deposit</td>
</tr>
</tbody>
</table>
The temperature along the spray evaporation surface was recorded with 28 different temperature probes during testing, see figure 16.

Figure 16: A display of the spray surface within the inner evaporation chamber of the Large Silencer. The red dots represent the locations of the temperature probes used during testing.

3.3 Numerical setup & method

**Scaling factor for specific heat** The recommended scaling factor (SF) for simulations of spray with the standard method in STAR-CCM+ is 10, which is used for all simulations.

**Time-step** A time-step sensitivity study was earlier performed for the Akvariet geometry by Emelie Trigell during a previous master thesis project at NXPS, Scania. This study recommends a time-step of 0.5 ms during injection of spray and 1 ms when there is no injection of spray [10, p. 29], which corresponds to a maximum Courant-number, \((C_{\text{max}})\) of 2 and 4, respectively. These values were implemented into an adaptive time-step function in STAR-CCM+, which was used to make sure that the CFL-condition, a necessary condition for convergence, was met at all times for all simulations. For a simplified one-dimensional case, the CFL (Courant-Friedrichs-Lewy) condition has the following form:

\[
C = \frac{u\Delta t}{\Delta x} \leq C_{\text{max}}
\]

where the dimensionless number \(C\) is called the Courant number, \(u\) is the magnitude of the velocity, \(\Delta t\) the time step and \(\Delta x\) the length interval.

**CFD Solver** All simulations are performed using STAR-CCM+ version 13.06.012-R8 double precision. The double precision is used to minimize errors with regard to rounding and to attain convergence within every time-step.
**Discretization** STAR-CCM+ uses a finite volume approach to represent and evaluate the partial differential equations that are solved every iteration. The spatial discretization is handled through the Hybrid Gauss - LSQ model. A second-order upwind scheme is used for the convective terms. A gradient limiter, called MIN-MOD, is utilized in order to hinder false oscillations. The temporal discretization is handled with first order accuracy for all simulations, as it was the only supported option for the Standard method.

### 3.4 Evaluation metrics for determining deposit risk

The metrics utilized for evaluating the formation of liquid film and thus the possibility of solid deposits forming are the liquid film thickness, liquid film mass and temperature of the spray evaporation plate. Furthermore, the footprint of the spray and the average and maximum liquid film thicknesses are also assessed when predicting the risk of solid deposit formation. The film mass source from the spray will be used for the investigations of critical parameters. For the frozen flow investigations, the assessment of the liquid film thickness requires more thorough means of analysis, and thus a standard area deviation is utilized:

\[
\sigma_{standard} = \frac{1}{N} \sum_{f} \frac{\sqrt{(\theta_{frozen} - \theta_{reference})^2}}{\theta_{reference} A_{cell - average}} A_{cell}
\]  

(33)

where \( \theta \) is the liquid film thickness of cell \( f \), \( A \) the area of the cell \( f \) and \( N \) the total number of cells. "Reference" stands for the reference case where the flow is never frozen and inner iterations are not changed.
4 | Results

4.1 Influence of critical parameters

This section presents the results obtained during the investigation of the influence of critical parameters. The following simulation results were all gathered from Akvariet simulations using flow condition case A (see table 2). If not explicitly mentioned as the investigated parameter, the following values were used for the investigations:

- number of parcel streams: 200
- volume refinement at the injector region: 0.5 mm
- number of inner iterations: 10
- frozen flow: no
- scaling of specific heat: none

Parcel Streams Increasing the number of parcel streams for the injection of AdBlue® spray yields higher computational times for each increment, as can be seen in table 5. The build-up of wall film mass along the spray evaporation plate during injection is reduced as the number of parcel streams is increased, as illustrated in figure 17. Furthermore, figure 18 shows how the film source from the spray becomes more evenly distributed as the number of parcel streams is increased.

Table 5: A display of how the computational time changes as the number of parcel streams is increased. Simulations are for one spray period (one second).

<table>
<thead>
<tr>
<th>Number of parcel streams</th>
<th>Computational time [hours]</th>
</tr>
</thead>
<tbody>
<tr>
<td>200</td>
<td>9</td>
</tr>
<tr>
<td>360</td>
<td>10</td>
</tr>
<tr>
<td>520</td>
<td>11</td>
</tr>
</tbody>
</table>
Mesh Refinement: Refining the cell size of the volume mesh at the injector region increases the computational time slightly for every step, see table 6. Figure 19 shows that further refinement of the injector region has a negligible effect on the generated wall film mass along the spray evaporation plate, with finer cell sizes only resulting in a marginally higher wall film mass. Additionally, from observing figure 20, no clear difference in the distribution of the wall film can be spotted as the cell size of the injector region is refined.

Table 6: A display of how the computational time changes as the volume refinement at the injector region becomes finer. Simulations are for one spray period (one second).
Figure 19: The wall film mass along the spray evaporation plate for the four different sizes of volume refinement at the injector region.

Figure 20: Distribution of wall film along the spray evaporation plate for the four different sizes of volume refinement at the injector region.

**Frozen flow** Simply freezing the momentum equations of the flow seems to have no effect whatsoever on the computational time, as shown in table 7. Reducing the number of inner iterations to three while the flow is frozen does however display a considerable reduction in the computational time, which is almost cut in half. Both cases that utilize frozen flow when allowed show only a slight deviation in the resulting wall film mass along the spray evaporation plate, as figure 21 shows.
Furthermore, the location and appearance of the produced liquid film remains highly similar between all three cases, as can be viewed in figure 22.

Table 7: A display of how the computational time and liquid film thickness area standard deviation changes as the momentum equations are frozen and inner iterations are decreased. Simulations are for ten spray periods (ten seconds). CII: constant inner iterations (10), VII: variable inner iterations (3-10).

<table>
<thead>
<tr>
<th>Case</th>
<th>Computational time [hours]</th>
<th>Standard area deviation [%]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Reference</td>
<td>102</td>
<td>-</td>
</tr>
<tr>
<td>Frozen - CII</td>
<td>102</td>
<td>0.847</td>
</tr>
<tr>
<td>Frozen - VII</td>
<td>56</td>
<td>2.751</td>
</tr>
</tbody>
</table>

Figure 21: A display of how the film mass at the spray evaporation plate deviates from the reference case as the momentum equations are frozen and inner iterations are decreased. CII: constant inner iterations (10), VII: variable inner iterations (3-10).

Figure 22: The liquid film thickness along the spray evaporation plate after ten seconds for the reference case, the frozen case with constant inner iterations (CII) as well as the frozen case with variable inner iterations (VII).
4.2 Influence of flow conditions

This section presents the results obtained during the investigation of the influence of different flow conditions.

4.2.1 Akvariet - test rig

The three different flow condition cases investigated for the Akvariet geometry and their respective deposit outcomes in testing can be seen in table 8.

Table 8: Data setup for the investigated cases of Akvariet. Temperature is the temperature of the flow at the inlet, dosing is the amount of AdBlue® being injected per minute through the injector. Deposit outcomes: *Pool = High amount of liquid film spread throughout the spray evaporation plate, Deposit = solid deposits appearing along the plate. **Approximate Reynolds number at the start of the evaporation system.

<table>
<thead>
<tr>
<th>Case</th>
<th>Temperature [°C]</th>
<th>Mass flow [kg/h]</th>
<th>Dosing [g/min]</th>
<th>Reynolds number** [-]</th>
<th>Deposit outcome in testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>180</td>
<td>400</td>
<td>5</td>
<td>5.7 · 10^4</td>
<td>Pool*</td>
</tr>
<tr>
<td>B</td>
<td>242</td>
<td>400</td>
<td>5</td>
<td>5.2 · 10^4</td>
<td>Deposit</td>
</tr>
<tr>
<td>C</td>
<td>275</td>
<td>850</td>
<td>10</td>
<td>1.06 · 10^5</td>
<td>None</td>
</tr>
</tbody>
</table>

Liquid film thickness For case A, figure 23 and figure 24 illustrate a continuous build-up of wall film thickness in the shape of a horse-shoe. The situation looks very different for cases B and C, as whatever amount of liquid film that is produced during injection seems to be immediately evaporated as the injection stops.

Figure 23: The average liquid film thickness along the spray evaporation plate for case A, B and C of the Akvariet geometry. Note the different ranges of liquid film thickness for each case.
Figure 24: The development of the liquid film thickness along the spray evaporation plate for case A, B and C of the Akvariet geometry. Note that the colorbar threshold for the liquid film thickness is different for every case.

Temperature comparison with test measurements As figure 25 suggests, the spray evaporation plate reaches lower temperatures for the physical measurements compared to the simulations for all cases. Looking at figure 26, it is evident that the largest temperature differences stem from probes 2-5 for all three cases.
4.2.2 Large Silencer

The three different flow condition cases investigated for the Large Silencer and their respective deposit outcomes in testing can be seen in table 9.

Table 9: Data setup for the investigated cases of the Large Silencer. Temperature is the temperature of the flow at the inlet, dosing is the amount of AdBlue® being injected per minute through the injector in relation to case F. Deposit outcomes: Deposit = solid deposits appearing along the plate. **Approximate Reynolds number at the start of the evaporation system.

<table>
<thead>
<tr>
<th>Case</th>
<th>Temperature [°C]</th>
<th>Mass flow [kg/h]</th>
<th>Dosing relative to case F</th>
<th>Reynolds number** [-]</th>
<th>Deposit outcome in testing</th>
</tr>
</thead>
<tbody>
<tr>
<td>D</td>
<td>230</td>
<td>450</td>
<td>0.13</td>
<td>4.0 \cdot 10^4</td>
<td>Deposit</td>
</tr>
<tr>
<td>E</td>
<td>350</td>
<td>1500</td>
<td>0.94</td>
<td>1.14 \cdot 10^5</td>
<td>None</td>
</tr>
<tr>
<td>F</td>
<td>350</td>
<td>1500</td>
<td>1</td>
<td>1.14 \cdot 10^6</td>
<td>Deposit</td>
</tr>
</tbody>
</table>

Liquid film thickness Figure 27 shows the build-up of liquid film thickness for case D, E and F of the Large geometry. Figure 28 shows a growing film thickness
for all three cases. For case D however, a large amount of the film that is produced every injection is evaporated before the next injection event starts, leading to a slower build-up of the film thickness. For cases E and F, most of the produced film is retained until the next injection event starts.

**Figure 27**: The development of the normalized liquid film thickness along the evaporation chamber for case D, E and F of the Large Silencer.
Average liquid film thickness

Figure 28: Normalized average liquid film thickness along the evaporation chamber for case D, E and F of the Large Silencer.

**Temperature comparison with test measurements** Figure 29 displays a rather good agreement between simulation and measurement when it comes to the averaged temperature along the spray surface for case D. Furthermore, figure 30 shows that the cold region of the spray evaporation surface for case D is placed in a similar location for both measurement and simulation, with the measurement reaching somewhat lower temperatures. For cases E and F, the averaged measured temperature in figure 29 is significantly higher than that of the averaged simulated temperature along the spray surface. Figure 30 provide further insight into this difference in temperature for case E and F, as the cold regions of the measurements only cover a portion of the even colder regions of the simulations. As the colder regions of a spray evaporation surface coincide with where the majority of the spray hits the evaporation surface, this indicates conflicting locations of spray hit between physical measurement and simulation for case E and F.

Average temperature by time

Figure 29: Normalized average temperature of all temperature probes along the evaporation chamber for both simulation and physical measurement for case D, E and F of the Large Silencer.
Figure 30: Normalized temperature along the evaporation chamber for both simulation and physical measurement for case D, E and F of the Large Silencer. The presented temperature data has been interpolated from the mean value by time for each temperature probe (seen as black dots placed throughout the evaporation chamber).
5 | Discussion

5.1 Influence of critical parameters

Regarding the influence of the number of parcel streams, figure 18 shows a clear difference in the distribution of the film mass along the spray evaporation plate between the three different cases. This is of high relevance for the speedup-method, which relies on a simulation consisting of only one spray period as its sole source of spray data for several spray periods. It is thus of vital importance that this spray data is as accurate as possible, which suggests that a high number of parcel streams should be used for the spray simulations of the speedup method.

Higher numbers of parcel streams also yield overall lower values for the wall film mass throughout the whole spray period (see figure 17). Figure 18 gives some hints as to why this might be. For the case of 200 parcel streams, the film distribution is very scattered and a few cells hold a tremendous amount of film compared to most of the cells of the spray evaporation plate. These cells thus become more cooled than the rest of the plate. Since the simulated time is only one spray period and the solid spray evaporation plate has thermal inertia, the cooler cells holding a lot of film attain a lower rate of evaporation. With the evaporation rate being lower, the film mass remain higher throughout the spray period for 200 parcel streams than for the other cases (see figure 17).

The increase in simulation time from increasing the number of parcel streams is rather small (see table 5). However, for cases with higher dosing of AdBlue®, the injection window becomes longer and thus the number of parcel streams starts to have more of an impact on the computational time.

On the subject of the refinement of the spray region, figure 20 shows no signs of there being any difference in the distribution of the film mass source from the spray between the different refinements. As seen in figure 19, the film mass only changes slightly as the cell size is refined. The change in computational time is also small (see table 6), as the refined cells only cover a small portion of the whole computational volume. However, the previously made argument regarding the computational time for higher dosing of AdBlue® holds true for the refinement of the injector area as well. Utilizing the refinement is thus rendered unnecessary for most dosing cases as computational resources is a limiting factor.

With respect to the simulations investigating the possibility of speeding up the solution by freezing the momentum equations, only the case where the inner iterations were variable (Frozen - VII) proved to actually reduce the computational time (see table 7). By reducing the inner iterations from ten to three for all instances where the momentum equations are frozen, the computational time was reduced by 45%. Freezing the momentum equations had a very small impact on the build-up of film mass along the spray evaporation plate for both frozen cases compared to the reference case (see figure 21). It is also worth noting that there is no accumulative
trend for either frozen case. Figure 22 shows the liquid film thickness along the spray evaporation plate after ten seconds. The pattern and position of the footprint of the liquid film remain very similar between all three cases. This is indicative that the process of freezing the momentum equations have not led to any significant differences in the movement of the liquid film, which in turn suggests that the flow was indeed rather steady during the time windows chosen for frozen flow. The low numbers of area standard deviation for the liquid film thickness seen in table 7 provide further support for this.

5.1.1 Recommended settings for the Akvariet geometry

From the results presented in figures 17-22 and tables 5-7, the following settings are recommended for the Akvariet geometry: Parcel streams: at least 400, preferably higher if possible. Volume refinement at injector region: deemed unnecessary. Frozen flow case: frozen with variable inner iterations.

5.2 Influence of flow conditions

Figure 23 shows the average liquid film thickness along the spray evaporation plate for the three flow cases displayed in table 8. Case A has a steady build-up of film (also seen in figure 24), which corresponds well with the deposit outcome of pool in physical testing. For case B and C, the evaporation rate of film seems to be noticeably higher, as any liquid film that is accumulated during the spray injections is immediately evaporated as the injections stop. A high evaporation rate leads to a higher concentration of gaseous isocyanic acid, which if sufficient can enable the formation of solid deposit. This corresponds to the deposit outcome of solid deposit for case B. Case C shows a similar pattern for the liquid film thickness in figure 23, but there are no traces of solid deposit in testing. Although the temperature and dosing are higher, the mass flow is also considerably higher for case C. It is thus possible that the dynamics of the short-lived liquid film are too high for any solid deposit to form for case C. A closer investigation utilizing the wall-film-dynamics equation (see equation (31)) throughout the simulation would however be necessary to provide more clarity into the situation.

Figure 25 displays the averaged temperature from all the temperature probes along the spray evaporation plate for both simulation and physical measurement for all three cases. All three cases illustrate an over-estimation of the plate temperature for the simulations compared to the physical measurements. Figure 26 shows that the biggest temperature differences between simulation and measurement exist for temperature probes 2-5. A quick glance at figure 12 provides us with the insight that the locations of these probes correspond to where the majority of the spray hits the spray evaporation plate, as can be seen in figure 24. The very same discrepancy between simulation and measurement can be seen for simulations performed in AVL Fire for the Akvariet geometry [27]. The Akvariet geometry is limited in its dosing performance, and thus all the physical measurements were made for low dosing cases. Since the injector has a constant injection
rate, the injection time becomes very short for low dosing. Injecting spray for such small windows of time generates more room for error, as any extra AdBlue® that is injected or otherwise entering the exhaust could quickly lead to a noticeable difference in the cooling of the spray evaporation plate. However, the difference in temperature between simulation and measurement seen in figure 25 is too large for injector inaccuracies to be the sole reason. The conductor of the physical measurements, Constantin Nottbeck, also points out other shortcomings of the Akvariet rig, such as: insufficient insulation and leakage through the window frames, which yield a lower evaporation performance than in simulations, where no energy losses to the surroundings due to leakage exist [26, p.45].

Large Silencer

Figure 28 shows the average liquid film thickness along the spray evaporation plate for the three flow cases displayed in table 9. All three cases display a growth of the liquid film thickness. However, the low dosing of case D makes the majority of the accumulated liquid film evaporate during every spray period. This high rate of evaporation leads to a high concentration of gaseous isocyanic acid, which has shown to be a major culprit in the formation of solid deposits. This thus correlates with the deposit outcome of solid deposit for case D found in table 9. Case E and F display different outcomes for solid deposit in physical measurement as the dosing is different and thus more urea is available in the resulting liquid film to form solid deposit for case F. In the presented simulation results for case E and F (see figures 28 and 27), there are no clear differences between the two cases that could hint on the onset of solid deposit. These cases would thus also require the use of the wall-film-dynamics assessment presented with equation (31) in order for the deposit risk to be evaluated properly.

Figure 29 displays the averaged temperature of all the temperature probes along the spray evaporation surface for both simulation and physical measurement. For case D, the correlation between simulation and measurement is quite good. The spray seems to hit the spray evaporation surface along its whole perimeter for both simulation and physical measurement (see figure 30). However, for case E and F, the temperature is under-estimated with regards to the physical measurements. A major reason for this disparity could be the difference in temperature displayed in figures 30 and 30. For the physical experiment, the majority of the spray seems to land in a region only covering half of the perimeter of the spray evaporation surface. Whereas for the simulations, the majority of the spray seems to land all around the whole perimeter of the spray evaporation surface, very much like that of case D.

There could be several reasons as to why the location of the spray hit seems to differ between simulation and physical test. First, there is the usage of the frozen flow approach. Although the location of the spray is correctly estimated for case D, it is possible that the frozen flow approach becomes more sensitive when the injection events become longer, which they are for case E and F (see table 9). After all, it was only validated for the Akvariet geometry for a case with a very short injection window. Further investigations of STAR-CCM+ for spray simulations will nonetheless be able to utilize the co-simulation approach, in which the frozen
flow approach is rendered unnecessary. Should the same discrepancy arise again without the use of the frozen flow approach, it might be worth to rerun the physical test. Both case E and F were part of the same test run (as they share the same temperature and mass flow), in which the dosing was increased in steps until solid deposit occurred. It is thus possible, although unlikely, that the angle of the injector or something else inside the test chamber was accidentally altered before this test began, resulting in the differently shaped spray hit that can be seen for case E and F but not case D in figure 30 for the physical measurements. However, there were more physical tests of high dosing cases performed on the Large Silencer geometry during this project. It would thus be more advisable to perform simulations on these cases and check whether or not the same issue of spray hit arise between simulation and physical measurement before conducting any more physical tests on the Large Silencer geometry. If the same problem still occurs without the use of the frozen flow approach, the repeatability of the experiments should be questioned.
6 | Conclusions

The following conclusions can be drawn from this project:

- The standard method for spray simulations in STAR-CCM+ has been implemented and tested for new parameter settings, including the use of freezing the flow for a potential speedup. Implementing the method is easy, user-friendly and the simulation process is robust and stable.

- Relevant parameters have been studied which are of good use for future implementation of the speedup method.

- Several operating conditions have been studied for two different geometries. Although the simulation results display some correlation with the physical measurements, more thorough assessments for identifying the risk of solid deposit has to be performed on the studied cases to attain a proper risk evaluation.

- There are differences between simulations and physical tests regarding the temperature of the spray evaporation surface. These discrepancies and the possible underlying reasons should be taken into account when performing further simulations and physical measurements in the future.
7 | Perspectives

The emission of pollutes such as $NO_X$ is damaging for the environment and deeply troublesome for densely populated cities. It is thus of highest importance to reduce these harmful emissions. Utilizing and further evaluating the methods investigated in this project can lead to a simulation arsenal that is more capable of predicting the risk for solid deposit and the correct mixing performance of ammonia in an evaporation system. This would in turn open up new possibilities when dimensioning the components of an aftertreatment system;

• Optimization of the UWS dosing, which helps
  – reduce the emission of excessive urea
  – increase the conversion rate of $NO_X$ in the SCR, thus reducing the emission of $NO_X$

• Optimization of the protection and resistance against component failure, increasing product quality and thus reducing waste and maintenance costs

Further development and validation of specifically the speedup method would also lead to lower lead times and thus development costs would be reduced. Additionally, the speedup method would make it possible to evaluate a larger number of configurations and concepts during a set amount of time. Hence, a higher number of promising designs would be available to choose from for experimental testing and prototype production. This could in turn lead to higher quality and performance of the finished product.
8 Future Work

This work has shed some new light onto the subject of simulating UWS spray for deposit prediction through STAR-CCM+. The investigated simulation method is continuously being improved and updated by Siemens, but there is still much work that lies ahead in validating the method for industrial applications on Scania silencers. The following areas are deemed the most relevant for future development:

- Fully implement and investigate the Co-simulation approach, which has the potential to speedup simulations considerably, thus also enabling further studies and investigations of the method to be performed more quickly.

- Performing a mesh sensitivity analysis on the large silencer geometry for the studied method.

- Investigate the wall-film-dynamics and other risk assessment tools for properly evaluating the risk for solid deposit.

- Perform simulations on the studied cases through AVL Fire for the purpose of comparing the performance of the different solvers.

- Carrying out simulations for other geometries.

- Executing simulations with the intent of performing a sensitivity analysis of the turbulence at the inlet (especially interesting for silencers with a pre-evaporator).

- Investigating the mixing performance of ammonia for the studied method.
References


A | Extended equations to the Fluid dynamics chapter

A.1 Transport equations for the realizable k-epsilon two layer turbulence model

Turbulence models that utilize the relation in equation (12) are called eddy-viscosity models. The model that is supported by the spray methods in STAR-CCM+ is the realizable $k - \epsilon$ two-layer turbulence model [2]. It solves two transport equations: that of the turbulent kinetic energy ($k$):

$$\frac{\partial}{\partial t} (\rho k) + \nabla \cdot (\rho k \bar{v}) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_k} \right) \nabla k \right) + P_k - \rho (\epsilon - \epsilon_0) + S_k$$ (34)

and the rate of dissipation of turbulence energy ($\epsilon$).

$$\frac{\partial}{\partial t} (\rho \epsilon) + \nabla \cdot (\rho \epsilon \bar{v}) = \nabla \cdot \left( \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \nabla \epsilon \right) + \frac{1}{T_\epsilon} C_{\epsilon 1} P_\epsilon - C_{\epsilon 2} f_2 \rho \left( \frac{\epsilon}{T_\epsilon} - \frac{\epsilon_0}{T_0} \right) + S_\epsilon$$ (35)

where $\bar{v}$ is the mean velocity, $\mu$ the dynamic viscosity, $P_k$ and $P_\epsilon$ are production terms, $\sigma_k, \sigma_\epsilon, C_{\epsilon 1}, C_{\epsilon 2}$ and $C_t$ are model coefficients (see table 10) and $f_2 = \frac{k}{k + \sqrt{\nu \epsilon}}$ is a damping function, in which $\nu$ is the kinematic viscosity. $S_k$ and $S_\epsilon$ are user-specified source terms and $\epsilon_0$ is the ambient turbulence value in the source terms with a specific time scale: $T_0 = \max \left( \frac{k_0}{\epsilon_0}, C_t \sqrt{\frac{v}{\epsilon_0}} \right)$, in which $C_t$ is a model coefficient.

From equation (34) and (35), the production terms are defined as:

$$P_k = f_c G_k + G_b - \Upsilon_M$$ (36)

$$P_\epsilon = f_c S_k + C_{\epsilon 3} G_b$$ (37)

where $C_{\epsilon 3}$ is a model coefficient and $f_c$ is a curvature correction factor.

Contributions to the production terms are:

Turbulent production

$$G_k = \mu_t S^2 - \frac{2}{3} \rho k \nabla \cdot \bar{v} - \frac{2}{3} \mu_t (\nabla \cdot \bar{v})^2$$ (38)
where $\mu_t$ is the eddy viscosity and $S = \frac{1}{2}(\nabla \bar{v} + \nabla \cdot \bar{v}^{T})$ is the mean strain rate tensor, in which $\bar{v}$ is the mean velocity.

**Buoyancy production**

$$G_b = \beta \frac{\mu_t}{Pr_t} (\nabla \cdot g) \quad (39)$$

where $\beta = -\frac{1}{\rho} \frac{\partial \rho}{\partial T}$ is the coefficient of thermal expansion for ideal gases, $T$ is the mean temperature and $g$ is the gravitational vector.

**Compressibility modification**

$$\Upsilon_M = \frac{\rho C_M k \epsilon}{c^2} \quad (40)$$

where $C_M$ is a model coefficient and $c$ is the speed of sound.

**Model coefficients**

<table>
<thead>
<tr>
<th>$\sigma_k$</th>
<th>$\sigma_k$</th>
<th>$C_{\epsilon 2}$</th>
<th>$C_M$</th>
<th>$C_t$</th>
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<td>1.2</td>
<td>1.9</td>
<td>2</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 10: Model coefficients for equations (14)-(15) and (36)-(40)

Furthermore:

$$C_{\epsilon 1} = \max \left(0.43, \frac{\eta}{5 + \eta}\right)$$

where $\eta = \frac{S k}{\epsilon}$

$$C_{\epsilon 3} = \tanh \left| \frac{v_b}{u_b} \right|$$

where $v_b$ and $u_b$ are the velocity components parallel and perpendicular to the gravitational vector $g$. 

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A.2 Wall treatment

$E'$ from equations (24)-(26) is defined as:

$$E' = \frac{E}{f} \quad (41)$$

where $E$ is the log law offset ($\approx 9.8$ for smooth walls) and $f$ is the roughness function [1]:

$$f = \begin{cases} 
1 & ; R^+ \leq R^+_{\text{smooth}} \\
\frac{B}{R^+_{\text{rough}} - R^+_{\text{smooth}}} + CR^+ & ; R^+_{\text{smooth}} < R^+ < R^+_{\text{rough}} \\
B + CR^+ & ; R^+ > R^+_{\text{rough}}
\end{cases} \quad (42)$$

where $B$, $C$, $R^+_{\text{smooth}}$ and $R^+_{\text{rough}}$ are model coefficients (see table 11), $R^+$ is the roughness parameter defined as:

$$R^+ = \frac{r \rho u_\ast}{\mu} \quad (43)$$

in which $r$ is a model coefficient, $\rho$ the density, $u_\ast$ the velocity scale and $\mu$ the dynamic viscosity.

and $a$ is an exponent defined as:

$$a = \sin \left[ \pi \frac{\log(R^+/R^+_{\text{smooth}})}{2 \log(R^+_{\text{rough}}/R^+_{\text{smooth}})} \right] \quad (44)$$

<table>
<thead>
<tr>
<th>$r$</th>
<th>$B$</th>
<th>$C$</th>
<th>$R^+_{\text{smooth}}$</th>
<th>$R^+_{\text{rough}}$</th>
</tr>
</thead>
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<td>0.253</td>
<td>2.25</td>
<td>90</td>
</tr>
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</table>

Table 11: Model coefficients for equations (42)-(44)

$P$ from equations (24)-(26) is a term that governs the velocity at which the log-law layer and the viscous sub-layer of the thermal profiles intersect [1]:

$$P = 9.24 \left[ \left( \frac{Pr}{Pr_t} \right)^{3/4} - 1 \right] \left[ 1 + 0.28 \exp \left( -0.007 \frac{Pr}{Pr_t} \right) \right] \quad (45)$$
References
