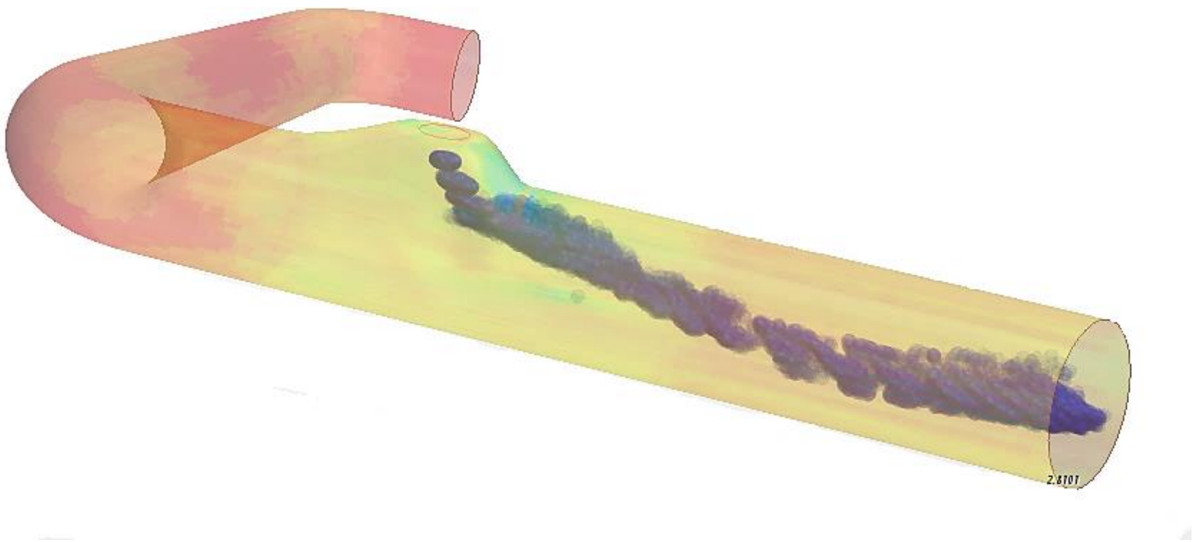

Methods for Urea Crystallization Analysis

A problem in reduction of NOx for the internal combustion engines

Master's thesis in Naval Architecture and Ocean Engineering

Naga Siva Sai Tarun Madisetty

DEPARTMENT OF MECHANICS AND MARITIME SCIENCES
NAVAL ARCHITECTURE AND OCEAN ENGINEERING

CHALMERS UNIVERSITY OF TECHNOLOGY
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Methods to analyze the problem of crystallization in reduction of NOx
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Cover:
[A definite analysis on the problem of urea crystallization in exhaust after treatment systems and methods to analyze them in advance.]

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SUMMARY

Volvo Penta is at present looking to improve the existing engines and to develop a next generation of engines. One of the main challenges with the present engines is the changes in the simulated exhaust flows and the backpressure developed due to the sedimentation of diesel exhaust fluids (DEF). This depends on various factors and parameters such as exhaust temperature, exhaust stream direction, DEF spray length etc. Therefore, a thorough research on this topic of DEF crystallization is useful to understand the behavior of the DEF in the exhaust pipes. The present report deals with the different phases of work involved in the methods that are developed to analyze the problem of Urea crystallization at Volvo Penta, Lundby, Göteborg.

The report is written in English.

Keywords: Urea, SCR catalyst, NOx reductions, Crystallization, NOx, Exhaust, Regulations.

Preface and Acknowledgement

As per the requirement to become a graduate in master's program of Naval Architecture and Ocean engineering, a master thesis have to be completed. Therefore, as a part of it the present thesis is taken up in the fourth semester of the program. The main objective of this thesis is to understand and analyze an existing industrial problem and provide conclusions based on the observations. The aim of the thesis is to propose and develop a method to understand the behavior of urea aqueous solution inside the exhaust pipe.

In order to achieve this concept, I would like to thank the following people for their time, interest, concern and guidance:

- Ivarsson Johan (Manager - Exhaust After treatment Systems, Volvo Penta) for sharing his insights, advices regarding the topics and help with providing required resources for the work.

- Nils Jansson (Design Engineer - Exhaust After treatment Systems, Volvo Penta) for his help on the whole thesis and his constant support which resulted in making the work easier in lot of situations.

- Lucien Koopmans (Professor / head of the division - Combustion and Propulsion Systems, Chalmers university) for his supervision for the whole thesis work and backing in difficult situations especially during Covid-19.

- Lönn Nina (Exhaust After treatment Systems Specialist, Volvo Penta) for her time and information about the problems that tend to result in crystallization and methods that can be worked on.

- Shreyas Dwarakanath (Calibration Engineer Fuel Systems, Volvo Trucks) for his interest and information on present developments in the exhaust systems and sensors.

- Abrahamsson Johan (Senior CAE Engineer (CFD), Volvo Group) for his help regarding the queries associated with the CFD models, and explanation of the processes followed.

- Razmjoo Narges (Test engineer, Volvo Penta) for her immense help in providing required test data for different engines and explaining the concepts involved.

- Ray Debdeep (Performance & Application Engineer, Volvo Trucks) for his detailed information on the calibration of NOx Sensors and their behavior.

- Yazdani Raman (Lead Engineer & Simulation Engineer, Volvo Group) for his explanation and ideas on flow bench and scaling the model concepts.

- Petter Dahlander (Professor at Chalmers, Internal combustion Engines) for his support in setting up the workstation and for his constant help when needed.

Description of the Task

Urea crystallization is a very common issue which can be noticed in the exhaust treatment systems which use UWS (Urea Water Solution) as their solvent for reducing nitrogen oxides emitted from the engine. Due to this crystallization there may arise problems like developing of backpressure, release of ammonia into the atmosphere, raised levels of NOx output etc. To, Volvo group which involves engines, exhaust and emissions in their main field of work, a thorough research or understanding of the interactions inside the exhaust pipe would be beneficial To look into this matter, a simple yet effective method to analyze this process of crystallization and evaluating different parameters and their effect on this phenomenon which can serve as a basis for understanding, to solve future problems or to design more efficient systems.

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Nomenclature

Functions and Scalars

ρ	[kg/m^3]	Density
hz	[sec^{-1}]	Frequency
ω	[m/s]	magnitude of rotation
D	[m]	Diameter of the particle
v	[m/s]	Velocity of the particle
σ	[N/m]	Surface tension
µ	[kg/m-s]	Dynamic Viscosity
L_a	-------	Laplace number
Rp	-------	Reynolds Number
R_{es}	-------	Shear Reynolds number

Abbreviations

AEM	Advanced Engine Modification
CAE	Computer Aided Engineering
CFD	Computational Fluid Dynamics
DEF	Diesel Exhaust Fluids
DPF	Diesel Particulate Filter
DWI	Direct Water Injection
EGR	Exhaust Gas Recirculation
FPS	Frames Per Second
NOx	Nitrogen Oxides (NO and NO_2)
SCR	Selective Catalytic Reduction
SLA	Stereolithography
STP	Standard Temperature and Pressure

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1. INTRODUCTION:

1.1. Emissions:

As the terms like environment, global warming, emissions, climate change, pollution, etc. are being stressed these days, the problems associated and incidents resulting in such conditions should be paid necessary attention. This focus on such problems resulted in more rules and regulations to be followed by automotive / marine industries and gave rise to more cut off levels in exhaust emissions to be achieved. There are several components of emissions that are harmful to the environment, humans, vegetation, and animals.

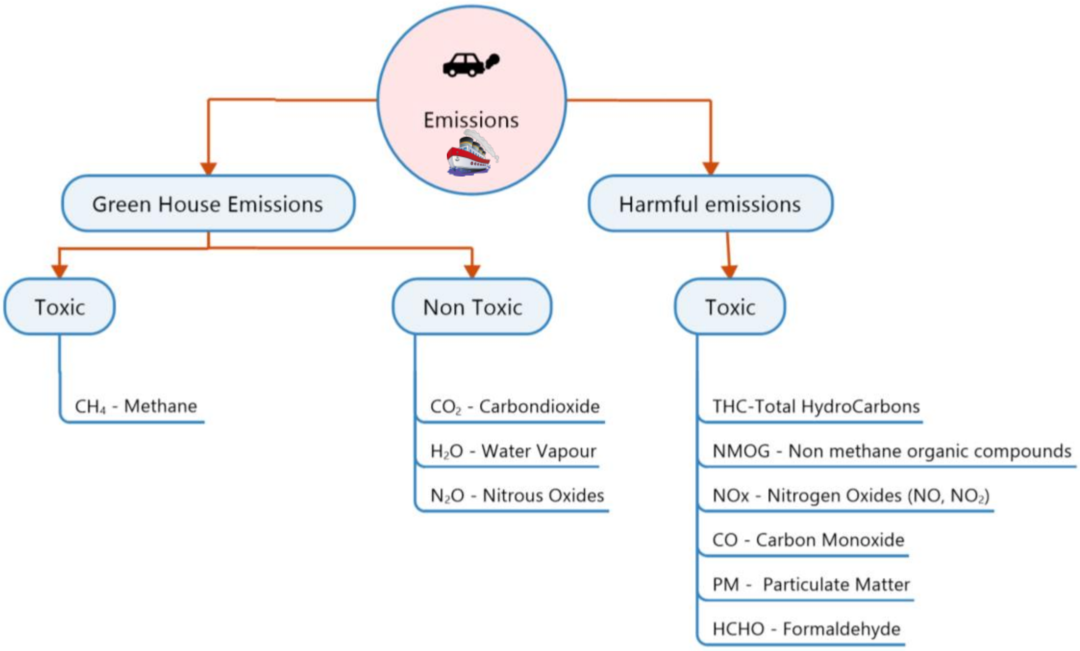


Figure 1: Classification of emissions

One such component of harmful emissions is NOx; NOx represents the nitrogen oxides (NO and NO_2) and is considered as a pollutant which can result in acid rains and smog. NO is a nontoxic element, but it is the forerunner of NO_2 which can cause emphysema and inhibit pulmonary defense. One of the primary sources for the release of NOx into the atmosphere is from the combustion engines and can be a major pollutant in high vehicle traffic regions. NOx requires higher peak cylinder temperatures in engine for an endothermic reaction to take place between nitrogen and oxygen molecules resulting in nitrogen oxides, these temperatures are favorable to occur in combustion engines during the combustion of fuels (hydrocarbons). Several methods are developed to reduce and filter out these emissions of NOx as much as possible. Methods like lean NOx trap and Selective catalytic reduction (SCR) are tested and proved effective in their own operating temperatures.

There are certain emission regulations set as a quantitative requirement to be followed by concerning countries. The limitation on NOx is gradually reduced through the past years and now the legislations in use are Euro 6 for cars in Europe and IMO tier III for sailing engines. These set of regulations are meant to be satisfied by every engine operating on-road and off-road. The limitations on NOx from engines after the exhaust after treatment systems are 0.08 g/km for the compression ignition engines, 0.06 g/km for the spark ignition engines and 3.4 to 2.0 g/kWh for sailing engines depending on the rpm.

To overcome the NOx abatement issue, several methods have been tried and tested in the past like Exhaust Gas Recirculation (EGR), Direct Water Injection (DWI), Advanced Engine Modification (AEM), Selective Catalytic Reduction (SCR) etc. Also other techniques such as choices of fuels, combustion control corresponding to reduction in peak temperature or reducing the gas residence in the high temperature zone or reducing oxygen concentrations, using low NOx burners (boilers), staged combustion (off-stoichiometric combustion) are well explained by *Bounicore, Anthony J., and Wayne T. Davis, eds. 1992* in their air pollution engineering manual.

Of all the mentioned, SCR (Selective Catalytic Reduction) technique is considered to be the most efficient way for NOx abatement *(Mathias Magnusson 2011)* in situations such as locomotives and other static engines. However, the SCR is an effective technique at high temperatures, since, NOx formation rises exponentially with increasing temperature *(Stultz and Kitto 1992)*, which is the region of substantial production of NOx by the engine.

SCR uses a spray of urea and water solution to produce ammonia gas using the heat in the exhaust, which reacts with the NOx present in the exhaust gases and reduce them to nitrogen and water vapor. However, if the temperatures are not enough for conversion of urea or if excess urea is released into the exhaust stream than required, there may be a possibility of urea crystallization in the exhaust pipes and near the spray modules. This would develop complications like increasing the backpressure or inefficiency in the conversion of NOx *(Lundström et al.2010)*. Therefore, to reduce the risk of inefficiency in the conversion of NOx to nitrogen, the concept of urea crystallization should be studied and analyzed. The prime focus of the thesis is to analyze the crystallization and to develop methods to examine and understand the occurrence of the urea crystallization. Further particulars of the study are described in the following chapters.

1.2. Volvo Penta NOx abatement technique and its working

1.2.1 Technique:

The same SCR technique discussed above is the most used method at Volvo Penta to reduce NOx, in this technique an external reducing agent in this case ammonia is introduced into the stream to react and reduce nitrogen oxides. The reducing agent ammonia is not stable and hence injected in form of urea and water mixture. Volvo allots some additional space in the system for this process to accommodate an AdBlue storage tank, and extra setup of catalyst in the exhaust stream. 'This technique sometimes can also lead to development of complications of crystallization and byproducts. *(Lundström et al. 2010).*

1.2.2 Working:

The SCR system consists of three major parts the AUS tank, the pumping unit and the SCR catalyst module (muffler).
The engine out exhaust which has high NOx concentrations is diverted into the exhaust pipes where there is an upstream NOx sensor either mounted on the engine or at the starting of the exhaust unit.
The exhaust pipe has a muffler unit consisting all the filters and reduction catalysts. A urea dosing valve is located before the catalyst which takes dosing input from the aftertreatment control module controlling the input frequency according


(a)
(a)

to the demand. The AdBlue solution is pumped into the dosing module with the help of a pumping unit Figure 2(a) and from a AdBlue solution holding tank. The tank has a sophisticated arrangement of level sensors and filtering units. The pump has a solenoid valve which pumps the remaining AUS fluid back into the tank when engine is shut down so that pipes are clean from crystals.

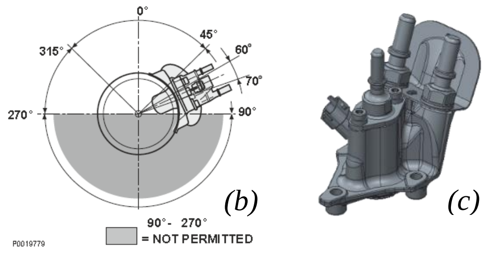


Figure 2: Components of injection system

It can be seen from the above Figure 2(b) that the urea dosage valve can be fixed anywhere on the injection pipe between 90° and 270° in order to protect it from condensed water after shutdown. The pre-temperature sensor before the dosing value gives the feed to control module which activates the dosing valve after reaching certain temperature. After the urea is injected and spread over the catalyst, catalyzed reactions occur between the exhaust and ammonia developed from urea decomposition. The fumes pass through a downstream NOx sensor present after the catalyst which analyses the NOx present and compare the error and adjusts the feed from the control module. The whole system can be found in the Figure 3 represented below.

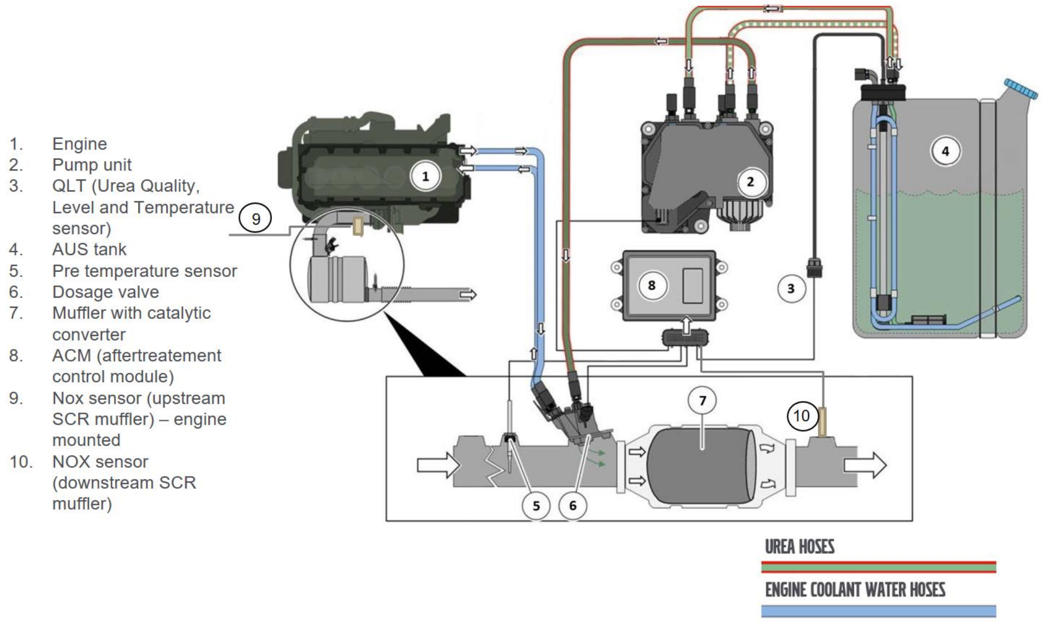


Figure 3: Complete representation of SCR

1.3. *Pre-Study*

The reduction of NOx in the exhaust occurs when the ammonia, which is released from decomposing of urea (AdBlue), reacts with the NOx to from nitrogen and water vapor. Ammonia is highly volatile in nature and exists in gaseous state at STP, here urea is used to decompose into ammonia and Isocyanic acid which further decomposes into ammonia and carbon dioxide. One mole of urea can be utilized to generate two moles of ammonia. There are certain reactions that occur in the exhaust pipe which lead to reduction of NOx. The urea is used in the system as an aqueous mixture of deionized water and urea generally known as AdBlue solution, Diesel Exhaust fluids or AUS32. This solution is primarily 32.5% Urea and 77.5% deionized water. This solution is injected into the exhaust stream containing NOx.

AdBlue / DEF / AUS32 →→ Urea $CO(NH_2)_2$ (32.5 w/w) + Water H_2O (77. 5 w/w)

Water in the aqueous mixture starts evaporating as the temperature is more than the boiling point which is a 100°C and urea starts decomposing at a temperature of 135°C and above. As the water evaporates from the UWS and since the temperatures are high the Urea remaining in the flow turns unstable and heated and starts to decompose. There are two types of reactions that occur in the decomposing of urea. Thermolysis reaction that occurs in exhaust pipe before the catalyst module and Hydrolysis reaction that occurs at the SCR catalyst module. *(Koebel, Elsener et al. 2000)*

H_2O (liq) + heat → H_2O (gas)… (Temperature > 100°C)

$(NH_2)_2CO$ + heat → NH_3 + HNCO… (Thermolysis of urea)

HNCO + H_2O (gas) → NH_3 + CO_2 … (Hydrolysis of HNCO)

A significant amount of energy is required for these reactions to occur, the source for this energy is only provided by the heat exchange from the exhaust gas and the wall surface of exhaust pipe. The heat exchange from the pipe wall to the AdBlue can cause a significant cooling of the pipe wall; cooling of several hundred degrees might occur especially if the AdBlue hits a small spot on the pipe wall for a long time which are commonly called as cold spots. *(Lundström A, 2010)*

The coagulation of the Isocyanate (HCNO) formed in the above mentioned thermolysis reactions can create a hard and insoluble compound (crystal) which needs a temperature above 350 °C to melt. This can happen if large amounts of non-hydrolyzed HCNO are present in the injection pipe. The cold spots mentioned above could be a perfect place to create temperature variation and thus leading to crystallization similar to the picture represented below in Figure 4.

Figure 4: Urea crystals developed during experimental studies at Volvo

There are certain reactions taking place between the ammonia (NH_3) released and NOx present in the exhaust stream which can be classified into three types that are rapid, moderate, and slow depending on the reactants involved and the time taken for reactions. *(Heck and farrauto.1995)*

NO + NO_2 + $2NH_3$ → $2N_2$ + $3H_2O$ … Rapid SCR reaction

NO + NO_2 + $2NH_3$ → $2N_2$ + $3H_2O$ … moderate SCR reaction

$2NO_2$ + $4NH_3$ + O_2 → $3N_2$ + $6H_2O$ … slow SCR reaction

Then the reacted flow passes through a slip catalyst which oxidizes any leftover ammonia in the stream. The nitrogen leaving would be diatomic along with water vapor. Overall, these above reactions in the exhaust stream at and before SCR helps reduce the NOx levels in the exhaust. More detailed discussion on decomposition is made by *H.L. Fang et al, M. Koebel et al, P.M Schaber et al* in their respective articles.

For this catalysis, a V_2O_5 catalyst may be preferred at temperatures ranging from 260°C to 450°C However, the catalyst used for the SCR completely depends on the operating temperature of the system. Platinum is used for low temperatures, vanadium for medium range temperatures and zeolites are preferred for high temperatures. *(Kröcher, O. et al. 2004)*

1.4. Inference from Pre-study

Some of the below mentioned trigger points are observed from studying the existing results at Volvo Penta and from observing the basic chemistry in the spray flow interaction which could be leading to crystallization in the exhaust stream.

a. Insufficient Surface Temperature: There are different behaviors of the spray droplets, when they hit the wall surface. According to different studies, they may adhere, evaporate, rebound, or spit. If the temperature is more than the Liedenfrost temperature the spray particles doesn’t touch the wall and there wouldn’t be heat loss occurring from the surface wall due to self-insulation of the droplet. If the surface temperatures are low, may be due to the turbulence or stagnation zones in the exhaust there may occur insufficient heat transfer to the particles making it hard for phase transition and as a result would lead to further cold spots.
b. Excess urea on the wall surfaces: There may sometimes be excess AdBlue solution released into the stream due to fluctuating temperatures in the engine and the fluctuating NOx sensor values respectively. This excess urea may lead to sedimentation in some cases.
c. Persistence of temperatures ranging from 150 °C to 200°C for longer duration : In some cold spots the temperature would be different from the whole system and if additional urea starts settling on the previously existing urea droplets then the core temperature of the stagnation will be less than the surface temperatures and at temperatures ranging between 150 °C to 200°C Cyanuric acid (an intermittent in the process of decomposing urea) starts coagulating and forms Crystals.
d. Less Area or specific area of contact by AdBlue: There may be chances where the spray is localized in a small surface due to the shape and flow velocities and there may be a localized cooling effect occurring due to this phenomenon.
e. Large droplet size of AdBlue: All the droplets in the spray are not in the same diameter and the probability of larger droplet size is never zero compared to the ideal droplet size. These large droplets require long time to evaporate water molecules in the droplet thus can decrease the system temperature for prolonged production of large droplets.
f. Slow catalyst light off : There’s certain temperature required in the exhaust flow for the catalyst to work, The catalyst light off time depends on the shape of the catalyst and the temperatures in the system, however there are sensors working to detect whether the light off temperature is achieved on not before releasing the urea stream, sometimes the whole ceramic catalyst may not be at the same temperatures in initial conditions and this may lead to crystals near the catalyst module.

1.5. Volvo Penta field test case-study

Volvo has their field tests with a D16-t4 final engine, it was observed that there is a slight crystallization at the AdBlue injector nozzle, however it is not a problem since it works as intended. The injection pipe looked like in Figure 5(c).

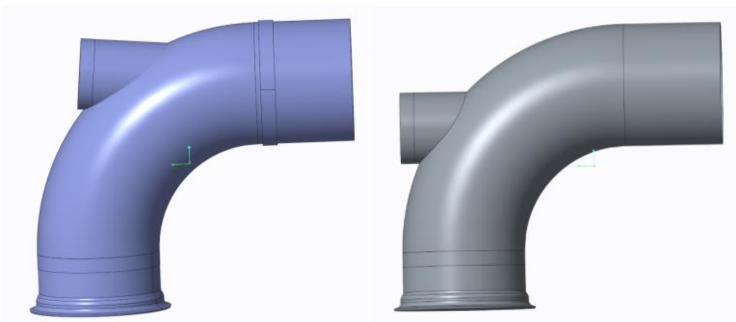
(a)Field Test vehicle *(b) D16-t4 engine* *(c)Injection pipe used*

Figure 5: Pictures showing the Field Test Vehicle, D16-t4 engine and the injection pipe

However, the same was tested for a stage-V engine and there seemed to be a huge buildup of crystals. This was tested in the engine rig with an AdBlue injection rate of 2 Hz and 16 hours of running. The huge buildup of crystals is shown in the below Figure 6.

Figure 6: Crystal buildup after 16hrs of running

To investigate this issue in further and to eradicate the above-mentioned problem, two new concepts were proposed. One to use the same design of u bent pipe but change the size of the injector nozzle and the other to change the position of the injector nozzle along with the size change. The proposed new prototypes are as shown in Figure 7 below.



Model (a) - increased injector boss size but same position (left)
Model (b) - increased injector boss with different position compared to old model (right)
Figure 7: New Proposed Models for testing

The new increased boss size showed a better spray without decreasing the temperature of injection boss due to decrease in continuous contact on the boss wall. However, there is a wall wetness observed due to tangential spray. This is rectified by changing the position of the injection boss making the flow mostly in the center of exhaust flow decreasing the wall-wetted surface thus reducing the temperature loss of wall.

Figure 8: Test results with 2 hz injection rate and 16hrs of running.

This technique of changing the spray position and injection pipe diameter has eradicated the problem in this case, but it may not always be favorable to use this kind of technique, since to test each and every experimental model on an existing engine setup would be really expensive. A flow bench which was in focus of this thesis study would be beneficial. However, the concept of the effect of flow on the spray and their respective shape and positions has a great effect on the crystallization is proved with a hard evidence in this case. The idea of designing the flow in a CFD which would be beneficial to study the flow and spray before hands was raised during going through the case of the field test. A special thanks should be mentioned to Nils Jansson (Design Engineer - Exhaust After treatment Systems, Volvo Penta) should be mentioned for explaining and demonstrating the whole case with necessary pictures.

2. OBJECTIVES AND ASSUMPTIONS

2.1 Objectives

Initially the objectives of the thesis were open, depending on the interests around the problem of crystallization. There were many ideas developed in the initial stage of the thesis to analyze the given problem in continuous discussion with the department of EATS at Volvo Penta. The prime ideas developed are presented below. Since, all of them cannot be carried forward basing on the timeframe and respective limitations.

- ❖ Design and development of practical flow bench test to see the interaction between the flow and the spray.
- ❖ Design simulations using a CFD software relating to the same above to investigate different cases beforehand to reduce costs.
- Develop methods to videotape the reactions and movements inside the exhaust pipe and muffler.
- Investigating optimal ratio between AdBlue hitting the wall and vaporizing in the stream and their relation to crystallization.
- Understanding the impact of different droplet sizes on crystallization.
- Investigating impact of swirl and standing waves on the mixing of spray.

The conditions by Volvo Penta are to develop a concept which can be utilized as a tool to analyze the urea crystallization beforehand. The method followed should be cost effective as much as possible, the ease of usage for further projects would be focused and the conditions generated should be resembling the operational environment. The first two ideas mentioned above are of utmost interest and sounded to fit in the boundary conditions.

2.2 Limitations

The thesis was initially planned to carryout experimental work to develop a flow bench or a cold flow rig and practically observe the spray behavior in the air stream resembling the exhaust flow without actually connecting the SCR muffler to the engine. But due to the issue of Covid-19 and the budgeting issues resulting as a consequence of Volvo group layoff. The scope of the thesis has been changed to CFD analysis of the same flow bench using the StarCCM+ software and to comparing with the existing test data at Volvo Penta.

The concepts developed for physical tests has been halted midway and the work that was done prior to the scope change is attached along with the report to help the future work and development in later stage.

2.3 Remedies

To overcome the issues as licensing and time, two cases from the experimental studies have been considered for the analysis. One case which showed heavy crystallization and the other with no crystallization at all.

The final objective of the thesis was set to perform CFD simulation of the specific cases of the performed experiments and see the relevancy to the experiments and use it as a tool for future practical experiments beforehand.

2.4 Assumptions

To reduce the computational time/power as much as possible for the simulations and to resemble the general working conditions of the experiments, some assumptions were made without disturbing the flow behavior, such as considering all the particles of the flow are spherical with a constant diameter which would decrease the computational power exponentially compared to considering the irregular shaped particles. However, the particle – wall, exhaust- spray interactions would still be like that of irregular particles.

The second one being that all the spray particles having a constant mass fraction (density) and temperature at the time of release, this has a little impact on the interactions between the particles when temperature regime is ON in Star-CCM+. However, the final simulations were done to check the wall wetting to check the resemblance with the experiments and this has a negligible effect in that case.

The third one is considering the exhaust flow to be non-pulsating, which would be a case in presence of the turbocharger, here the considered time frame of the simulation is quite small and hence the impact is negligible.

The fourth being the impurities and other particles were not considered along with the gaseous mixture, since defining their chemical and physical properties and designing such particle would only complicate the work than to obtaining improved results.

The fifth being that the variation in the ambient temperature (rise or fall of temperature in the surrounding) has very less effect on the system, whereas there wouldn't be much variation in the ambient temperature anyway in such small simulation time.

The sixth assumption is that the mixture of exhaust gases is assumed to possess ideal gas behavior and with correction for cP=cP(T) from NASA thermodynamic table for Star-CCM+ which means that the gas particles present in the system are considered as point particles with random movement but with no inter particle interactions.

The seventh one of the assumptions being that there is no consideration of change in the backpressure in the system this can be considered constant considering the time frame of the simulation.

Eighth assumption is that the model is considered to obey k-Ω SST (shear stress transport) turbulent model, with default damping factors and coefficients. Since, k- ε model predicts good in the region far from the boundaries (wall) and k- Ω model predicts well in near wall regions. An SST model is considered which is basically a combination of both.

The ninth assumption is that the particles in the system only possess translational motion and doesn't rotate, this is to minimize computational power as the particles doesn't change their direction of movement even if they rotate, hence the direction of movement of the particles is almost the same with and without this assumption.

Tenth assumption is that with a 2nd order implicit time discretization, the courant number may exceed unity. Here implicit method finds a solution by solving an equation involving both the current state of the system and the later one. Using a second-degree equation would sometimes lead to courant number being greater than one in some places of the system. Courant number is a number refers to the timestep that can be used, with the help of timestep function in Star-CCM+ it can be checked whether it satisfies Courant-Friedrichs-Lewy (CFL) condition which is

$$C = \frac{\mu \delta t}{\delta x}$$

Where C is called the Courant number, u is the velocity magnitude, Δt is the time step and Δx is the length interval.

The final important assumption is that the virtual mass force in the system is neglected. Virtual mass or added mass of the system is inertia added to the system as a body moves some fluid around it while the body is in motion. Neglecting these added mass components for the particles makes the timesteps to solve faster and requires very less computational power required comparatively.

All the above mentioned assumptions are chosen in the software and modified such that they have the slightest effect on varying the results from the original, However the relevancy can be checked by comparing the simulations with the experimental data and results in possession.

3. CFD DESIGN

Different tests that are previously conducted at Volvo Penta are studied and different parametric values are noted to evaluate any correlation between the data. Parameters such as Temperatures, Exhaust flow rates, Urea flow rates, Speed, Torque and power of engine, amount and weight of crystals formed, NOx levels after engine and SCR are readily available from the experimental data. Both the D8 and D16 engines of Volvo are tested for crystallization but however D8 was tested for different prototypes of injections pipes. Hence, test data of D16 was considered for further analysis. Most of the tests are run for 15 hours and the tests, where there is high crystal development are considered as major points for CFD analysis.

For the design of the same in the CFD, a setup of similar flow conditions as the experiments is to be designed and to achieve this, parameters such as temperatures, exhaust flow rate and urea flow rates are considered from the above experiments.

3.1 Modelling

3.1.1 Design:

The 3d models of the injectors are available at Volvo Penta in Creo and can be exported to mostly any 3d file format. But however, the models are not CAD cleaned for the meshing to be accurate. Instead of importing the models creating a model with required extensions on sides in any CAD software would both save time and work. For this thesis initially cad cleaning the imported models was tested.

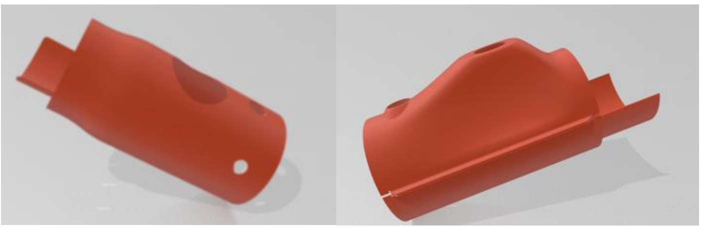
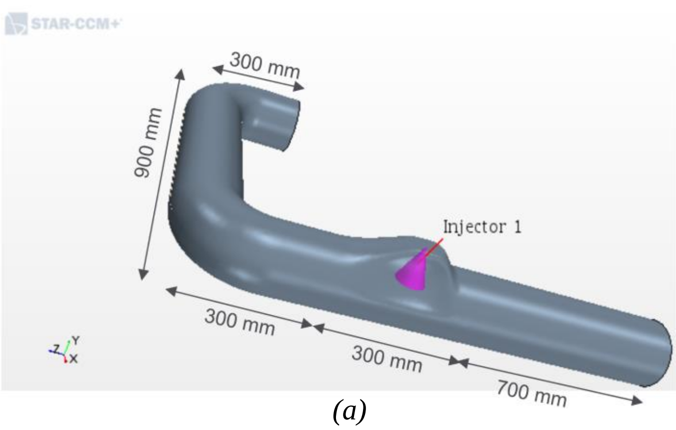
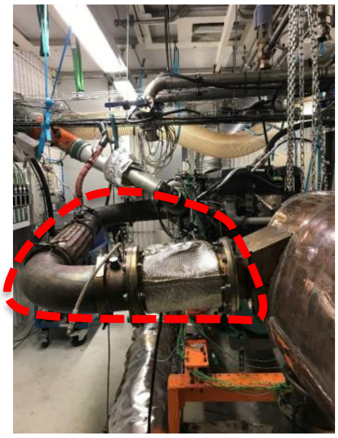


Figure 9: 3D models available in Creo.

Since, the end results of the model are not satisfactory, a whole new surface model was generated using AutoCAD 2020 and Rhino-6 3d. Points from the same surfaces in Figure 9 are used to generate a new 3d surface with exhaust pipe extensions on both sides to resemble similar to the pipe used in the experiments.



(a)



(b)

Figure 10: 3D developed in AutoCAD(left) , actual experimental setup with engine (right).

The total flow length, as can be seen from the Figure 6(a) is 2500mm (2.5 meters), including an extension of 700mm that is added after the injection module to observe the spray behavior and point of contact on surface. The point of interest is added after 700mm because the experiments performed by Razmjoo Narges (Test engineer, Volvo Penta) showed most of the crystal developments over this place and the region is not easy to access and difficult to take pictures of the crystals and measure them quantitatively. The picture in Figure 6(b) represents the actual setup on which respective experiments are performed relating to the experimental data in possession. The pipe marked in red dotted lines is the one in design focus.

3.1.2 Meshing:

Initially a coarse mesh was used but was found to be not accurate in solutions and likewise for the convergence of solution. A finer mesh size was used below are the details of both the meshes used. However, as the mesh becomes fine the computation time for each timestep slightly increases. But it’s a tradeoff that should be agreed to get accurate results.

Course mesh: The base size of the polyhedral meshing is set to 10mm, and finer mesh of sizing 50 percent to base size (5 mm) is used in required regions such as over the spray module. The achieved Courant number is less than one (unity) in most of the domain. The total numbers of cells are around 400000. And the time step used for the analysis was 0.25 milliseconds.

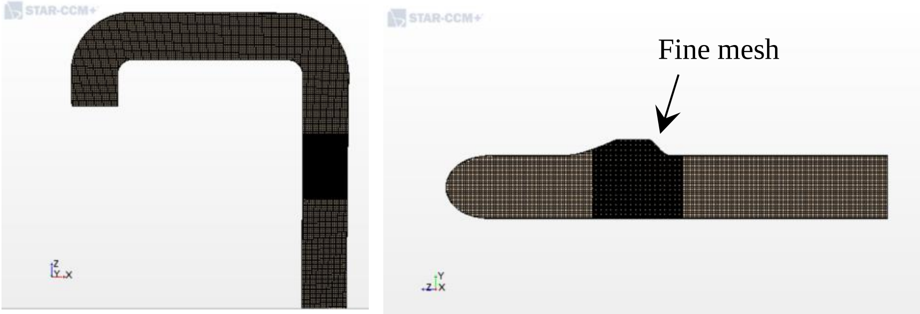


Figure 11: Course mesh- sectional cut top view (left), sectional cut side view (right).

Fine Mesh: The base size of the polyhedral meshing is set to 4 mm, and finer mesh of sizing 30 percent to base size (1.2 mm) is used in required regions such as over the spray module, inlet and exhaust. The achieved Courant number is less than one (unity) in most of the domain. The total numbers of cells are around 7730500. And the time step used for the analysis was 0.01 milliseconds.

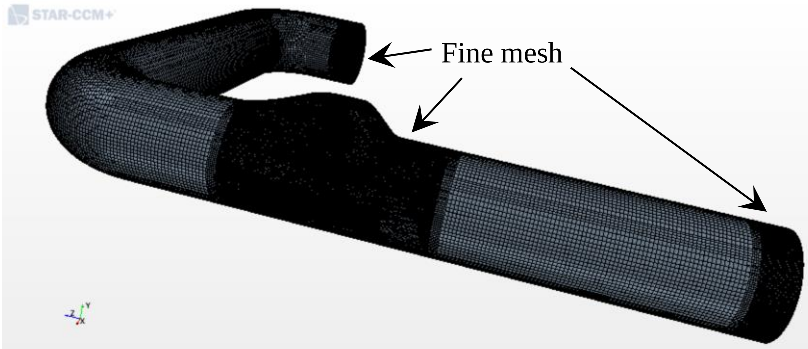


Figure 12: Fine mesh perspective

Courant number – Courant number refers to the timestep that can be used, with the help of timestep function in Star-CCM+ it can be checked whether it satisfies Courant-Friedrichs-Lewy (CFL) condition which is

$$C = \frac{\mu\delta t}{\delta x}$$

Where C is called the Courant number, u is the velocity magnitude, Δt is the time step and Δx is the length interval.

3.1.3 Injectors:

A solid cone injector from the available options is designed at the same position as shown in Figure 6 (a) in page 9. The spray data from Bosch ETI-5 (B280436700-03) @ 9 bar with six nozzle holes is considered. The spray angle is 42° with initial droplet velocity of 32 m/s and average droplet size of 71µm. Hence, using the density of AdBlue solution and average droplet size. If the urea flow rate of the experiment is known, then the number of particles (N) can be estimated and can be used for setting the parcel stream value.

3.1.4 Critical Parameters:

Parcel streams – The time consumed by the simulations would be very high if it has to solve equations for every possible particle in the flow. Parcel streams which act as a group of particles and would reduce the computational time and power. But deciding the number of parcel streams to be used also needs to be analyzed as the number of parcel streams increases the time taken increases exponentially. For this thesis, parcel size of 300 is used for ease of computation and moderate accuracy of results.

Inner Iterations – The number of inner iterations is set to 15 as optimum.

Mesh refinement – The mesh is refined at injector module with base size of 1.2 mm.

Wall temperature – A fixed wall temperature is set depending on the respective experimental data.

3.2 Physics:

The conservation of mass, momentum and energy are the main physics involved in performing the simulation analysis for this thesis. Fluid behavior or the pattern of movement can be studied or interpreted through numerical calculations by utilizing the rules of conservation and making some valid assumptions to simplify the physics.

3.2.1 Drag component:

To determine whether the flow is laminar, turbulent or a mixture of both, a dimensionless entity is used called the Reynolds number. It is given as the ratio between inertial forces and the viscous forces in play.

$$R_p = \frac{Inertial\ forces}{viscous\ forces} = \frac{\rho v l}{\mu}$$

Where Rp is the Reynolds number corresponding to the particles in the flow, ρ is the density of the fluid in (kg/m3), v is the velocity of the fluid in (m/s), l is the characteristic linear dimension (m) and μ is the dynamic viscosity of the fluid (kg/m-s).

Since the Lagrangian approach (*Lagrangian approach is where the individual particles are noted and their properties like positions, directions, velocities etc. are expressed with respected to a unit of time, and all the laws of physics and principles of conservations are applicable to each noted particle individually*) is being used for the modelling, there are two options available for the prediction of drag model of the particle in Star-CCM+.

a. Sciller-Naumann model:

$$C_d = \begin{cases} \dfrac{24\left(1 + 0.15R_p^{0.687}\right)}{R_p} & R_p \leq 1000 \\ 0.44 & R_p > 1000 \end{cases}$$

Here C_d is the drag coefficient and Rp is the Reynolds number of the particle.

b. Liu model:

$$C_d = \begin{cases} \dfrac{24(1 + \frac{1}{6}(R_p^{2/3}))}{R_p} & R_p \leq 1000 \\ 0.424 & R_p > 1000 \end{cases}$$

Here C_d is the drag coefficient and Rp is the Reynolds number of the particle.

For this study the Sciller-Naumann model has been used. This model has a separate shape deformation factor included for the particle which is considered useful after comparison with the liu model, and the shape deformation factor is given as

$$C_d = C_{d(spherical)}(1 + 2.632y)$$

Where y is a non-dimensional number that is used to represent the expansion of the effective diameter of a particle. It is used mainly for the drop distortion and break-up modelling.

3.2.2 Lift components:

In the Lagrangian approach, there are two options available for the prediction of shear lift force of the particle in Star-CCM+.

a. Saffman method: This method can be applicable to low range of R_p.

$$C_{SLF} = \frac{4.1126}{R_{es}^{0.5}}$$

Here C_{SLF} is the lift coefficient and R_{es} is the shear Reynolds number and is defined as

$$R_{es} = \frac{\rho/\omega/D^2}{\mu}$$

Where ρ is the density(kg/m3), /ω/ is the magnitude of rotation(m/s), D is the diameter of the particle (m), μ is the dynamic viscosity of the fluid (kg/m-s).

b. Sommerfeld method: This method can be applicable to broader range of R_p

$$C_{SLF} = \frac{4.1126}{R_{es}^{0.5}} f(R_p, R_{es})$$

Where $f(R_p,R_{es})$ is the correlation for higher Reynolds number proposed by *Mei (1997).*

For this study Sommerfeld method has been used since the Reynolds number range is much broader and the correlation factor shows better values in high speed and low viscous flows. *(P.G Saffman, 1965) (Sommerfeld,1998)*

3.2.3 Wall droplet interactions:

A model that would contain and calculate most of the droplet behaviors as a consequence of impingement on the wall surface would be beneficial for the study. There are two possible models for this type of wall bounded flows.

a. Bai-Gosman model: This method uses the weber number of the particle W_{ep} and T_w with T_{Boil} and $T_{Leidenfrost}$.
   Here T_w, T_{Boil}, $T_{Leidenfrost}$ are temperature of the wall, boiling and Liedenfrost temperatures respectively and W_{ep} is defined as $W_{ep} = \frac{\rho D v_{r,n}^2}{\sigma}$; where $v^2_{(r,n)}$ is the relative velocity of particle, σ is the surface tension.
b. Bai-Onera model: A modification to Bai-Gosman that is developed to smooth results when $T_w < T_{Boil}$ and uses the Laplace (L_a) number which is defined as $L_a = \frac{\rho D \sigma}{\mu}$.

For this study Bai-Gosman models are used. There are certain outcomes that can be captured using this wall impingement model like adhere, rebound, spread, breakup and rebound, breakup and spread, splash. The representation of the model can be seen in the below Figure 13.

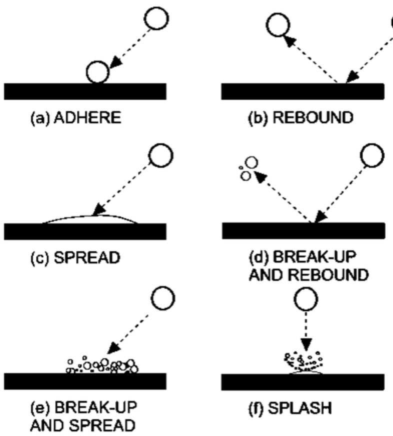


Figure 13: Captured outcomes of Bai-Gosman models

Adhere is where the particles stick to the surface, Rebound is where they reflect from surface and the path gets tracked, spread is where the droplets breaks into a fluid film on the surface, Breakup and rebound is where the droplet divides into finer droplets upon hitting the surfaces and the finer particles bounces back, Breakup and spread is when the finer particles form a liquid film, splash is when droplets breaks into smaller particles and few of them reflect in the same direction. *(Bai and Gosman, 1995).*

3.2.4 Turbulence*:*

Since its highly impossible to solve the governing equations analytically in cases like this. Hence to simplify the equation or to solve them, simulations are developed using mathematical models. There are different approaches to deal with the turbulence in a simulation. Direct numerical simulations (DNS) which solves turbulence of all scales but requires immense computational power. Large eddy simulations (LES) can be used or initial low scale turbulence which is not suitable for this study. Reynolds Averaged Numerical simulation (RANS) are the best way to predict the motion of fluid using time averaged equations in flows similar to this. Since the present study is implicit unsteady (flow changes with respect to the time), the URANS (Unsteady Reynolds Averaged Numerical Simulation) method can be used in this type of situation. The URANS methods adds a transient unsteady term (turbulent fluctuation) to the existing time averaged and fluctuation terms from RANS method. Time averaged components are still a prime focus even though the flow is unsteady. (*Davidson L. (2015)).*

The RANS model can be depicted as

$$\upsilon = \ddot{\upsilon} + \upsilon'$$

Here if υ is considered as a parameter of interest that is time dependent, $\ddot{\upsilon}$ is the time-averaged component and υ' is the resolved fluctuating component.

The URANS model can be represented as

$$\upsilon = \ddot{\upsilon} + \upsilon' + \upsilon''$$

Where υ'' is the modelled turbulent fluctuation which is unsteady.

With the help of this model and by following/satisfying the rules of conservation, a simulation model can be developed to represent the necessary flow conditions.

3.2.5 Near Wall Behavior:

Due to the viscosity of flow, there is resistance developing as a result of it. Defining the flow close to the wall boundary or the flow that is affected by the boundary layer has a great effect on modelling the flow. There may be vortices developing or deviation in the flow pattern observed due to wall interactions. In fluid mechanics regime, the thin viscous influenced layer near to the wall surface (boundary layer) can be divided into four regions further. *(Versteeg HK, Malalasekera W., (2007))*

a. Viscous sublayer
b. Buffer layer
c. Logarithmic region
d. Wake region

The thickness of these regions is represented by using a non-dimensional unit y^+, the velocity is represented by using a non-dimensional unit u^+, which are used to define the distance from the wall and velocity of the flow over that distance and are defined as follows.

$$y^{+} = \frac{y u_T}{v}$$

$$u^{+} = \frac{u}{u_o}$$

Here u_T is the velocity of fluid near wall or friction velocity, y is the distance from wall surface, ν is the kinematic viscosity, u is the actual velocity of fluid. *(Chanson, H. (2009)).*

The following Figure 14 can be used to depict different regions accordingly.

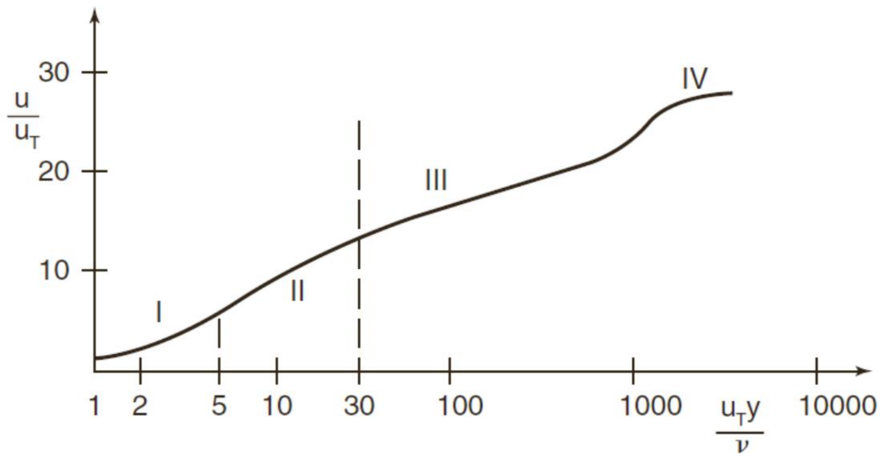


Figure 14: Near wall viscous regions

a. Viscous *Sublayer:*

In the turbulent boundary layer, this layer has a linear increase between u+ and y+ since it is the closest layer to the wall and is highly dominated by viscous forces. In this region $0 \le y+ \le 5$ and $u+=y+$.

b. Buffer Layer:

This is the transition region where the region slowly transits from having a linear relationship to a logarithmic relation. The range of y+ is from $5 < y+ < 30$.

c. Logarithmic region:

The forces of inertia play a crucial role in this layer. The value of y+ is as following $30 \le y+ \le 500\text{−}10000$, and the u+ is given by a log equation $u^{+} = \frac{1}{k}\log(y^{+}) + C$. Here κ is the von Kármán constant and generally takes the value of 0.41 and C has a value of 5.

d. Wake Region:

In this region a wake function is added to the above logarithmic region and exists after the log law region and the end of boundary layer. The wake function is denoted by $W(\frac{y}{\delta})$ and the equation for u+ is given as $u+= \frac{1}{k}\log(y^{+}) + \frac{\pi}{k} W\left(\frac{y}{\delta}\right) + C$.

The y+ values are always observed throughout the simulations to understand the boundary layer development around the inner surface of the wall.

3.2.6 Other models and options:

Liquid properties such as density, surface tension, and viscosity are keyed in as a polynomial of the temperature with values which are made available online.

Turbulent particle dispersion model is enabled, as the number of particles is already high, and this stochastic approach invented by *Gosman and Ioannides (1983)* can be used in this case. But however, the computational power and time increases accordingly.

Taylor Analogy Break-up (TAB) option for breaking or decomposing of a particle into respective child particles is available, this option is useful for using the effect of expansion in size of a particle and subsequent separation. Accounts for expansion of effective diameter and eventual separation.

3.3 Simulation setup

The simulation is setup by defining necessary properties and choosing the options that are suitable and would work according to the requirement. The properties below are a necessary to be defined in Star-CCM+ for simulation to converge and for ease of simulation.

a. Physics Continuum: The following are the properties set to define the physics of the simulation
   Properties: Implicit Unsteady, 3-Dimensional flow, Multi-component gas, Lagrangian Multiphase, Turbulent Flow, Turbulence suppression, Reynolds Averaged Navier Stokes (RANS), k-Omega shear stress turbulence, Non-reacting particles, Gravity, Segregated flow, Low y+ wall Treatment.
b. Spray model (Lagrangian Multiphase): The spray model is chosen to be the following: Multi-component Liquid, Spherical Particles, Material Particles, Constant Density, Virtual Mass, Parcel Depletion, Boi-Gosman Wall Impingement, NTC Collision Model, Turbulent Dispersion, Two Way Coupling, Drag Force, TAB Distortion, TAB Breakup, Quasi-Steady Evaporation.
c. Multi-component Gas: The exhaust is designed as a Multi-component gas with the following compositions.
   Composition: Water Vapour (H_2O -2.5 %), Nitrogen (N_2-77.5%), Oxygen (O_2-16%), Carbon dioxide (CO_2-6.25%).
d. Multi-component Liquid: The spray module is designed as a Multi-component liquid with the following compositions.
   Composition: Water (H_2O -77.5 %), Urea (32.5%)

4. RESULTS

Due to limited time and resources such as availability of licenses for Star-CCM+ two cases are chosen for the simulation process.

Test 1 was conducted on D2 P50 cycle for 15h with forced urea 0.862 (g/s) with SD10 fuel.

Test 18 was conducted on E2 P25 cycle for 15h with forced urea 0.32 (g/s) with SD10 fuel.

The crystal level is given in ranges of 0 to 3 where Level 0 indicates tiny amount or traces of crystals which often appear and disappear within minutes and are hence not considered as a risk for crystallization. Level-1 indicates some thick crystals in size but can still be neglected as they do not impose any risk on the system or the flow. These crystals are negligible when compared with the cross section of the exhaust pipe. Level-2 indicates a considerable amount and size of crystal which are not very large but still has a little effect on the flow or the engine which may result in particulate matter or power losses etc. Level 3 indicates large crystal growth with a direct effect on engine including power losses, backflow etc. these crystals give a scope or margin for additional growth of crystals, a crystal that is larger than level to can be categorized as a level-3 crystal. Pictorial representation of the levels of crystallization are mentioned in the appendix- Figure iii.

The crystals in Test 1 are level 0 and the crystals observed in test 18 are level-3

Test- 1	**Date**	**Cycle**	**Hours**	**Fuel**	**Speed, Torque**	**Exhaust flow (kg/s)**	**sectional area m^2**	**T_a Turb (C)**	**T_b_ SCR (C)**	**SensVal DPF Temp or calculated**
	11-10-2019	D2 (1800 rpm) P50	15	SD10	1800 rpm, 1539 Nm	0.563	0.017	NA	312	313
	urea flow (g/s)	**Urea flow/Exhaust flow**	**Forced**	**Power (Kw)**	**Amount of crystals**	**Crystal Level**	**Weight of crystals (g)**	**Conversion**	**SO Nox**	**EO Nox**
	0.862	1.531	Yes	290	No crystals	0	not removed	70.20	2.20	7.37

Table 1 : Table with data from Test -1

Here T_a Turb is the temperature after the Turbocharger, T_b SCR is the temperature before SCR, SensVal DPF is the Sensor temperature value at DPF, SO NOx is the SCR out NOx, EO NOx is the engine out NOx, Conversion is the ratio between SO NOx and EO NOx.

Test- 18	**Date**	**Cycle**	**Hours**	**Fuel**	**Speed, Torque**	**Exhaust flow (kg/s)**	**sectional area m^2**	**T_a Turb (C)**	**T_b_ SCR (C)**	**SensVal DPF Temp or calculated**
	2019-12-03	E2 (600 hp) P25	15	SD10	1800 rpm, 585 Nm	0.367	0.017	249	241	236
	urea flow (g/s)	**Urea flow/Exhaust flow**	**Forced**	**Power (Kw)**	**Amount of crystals**	**Crystal Level**	**Weight of crystals (g)**	**Conversion**	**SO Nox**	**EO Nox**
	0.32	0.8719	Yes	110.35	Much crystal in the SCR pipe	2 or 3	not removed	76.13	1.46	6.1

Table 2 : Table with data from Test -18

As the cross sectional area of the pipe is known it can be used to calculate the exhaust flow in metre/sec which is a needed input for the inlet flow in Star-CCM+, the urea feed is given in g/sec for the spray model, Temperature before SCR is taken as the temperature of the wall surface

Test 1 – Exhaust Flow = 0.563 kg/s

Sectional Area = 0,017 m^2

Density of Exhaust at 312°C = 0.58 Kg/m^3

Velocity of the exhaust flow $= \frac{0.563}{0.017\ x\ 0.58} = 56.42\ m/s$

Test 18 –Exhaust Flow = 0.367 kg/s

Sectional Area = 0,017 m^2

Density of Exhaust at 312°C = 0.68 Kg/m^3

Velocity of the exhaust flow $= \frac{0.367}{0.017\ x\ 0.68} = 31.37\ m/s$

Taking all the values from the experimental tests as inputs and defining the material properties of all the gases and liquids involved as a polynomial with respect to temperature, different properties are modelled in different scenes and the same are observed for the main differences between the two tests and the particle velocity is considered as the main evaluating principle to find the stagnation points in the exhaust pipe.

The simulation is run for a physical time of total 1.0 second

The Test - 1 results are shown in the following page at different solution times in the following page with urea input as 0.862 g/s, wall temperature as 315°C, exhaust flow rates as 56.42 m/s.

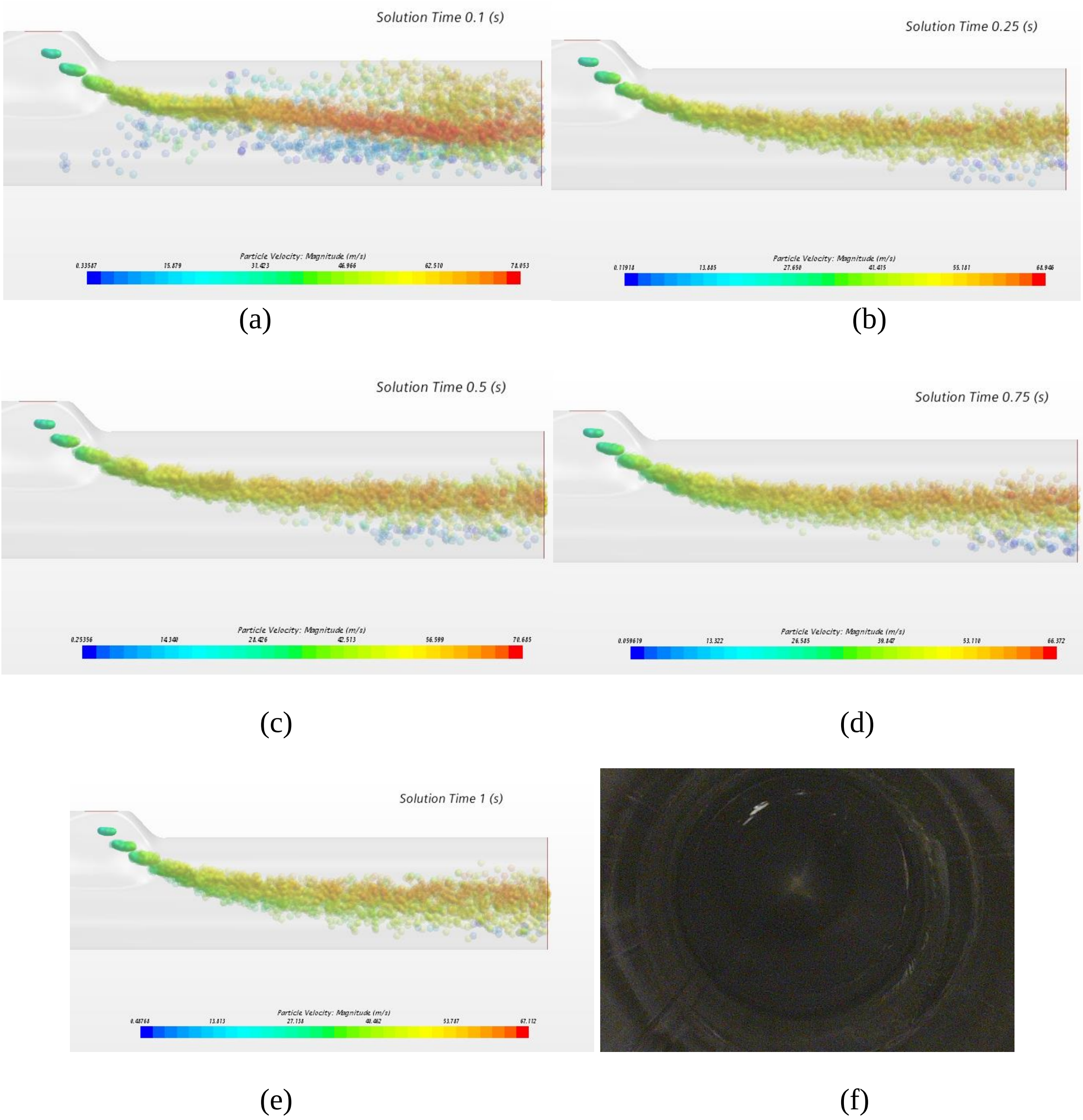
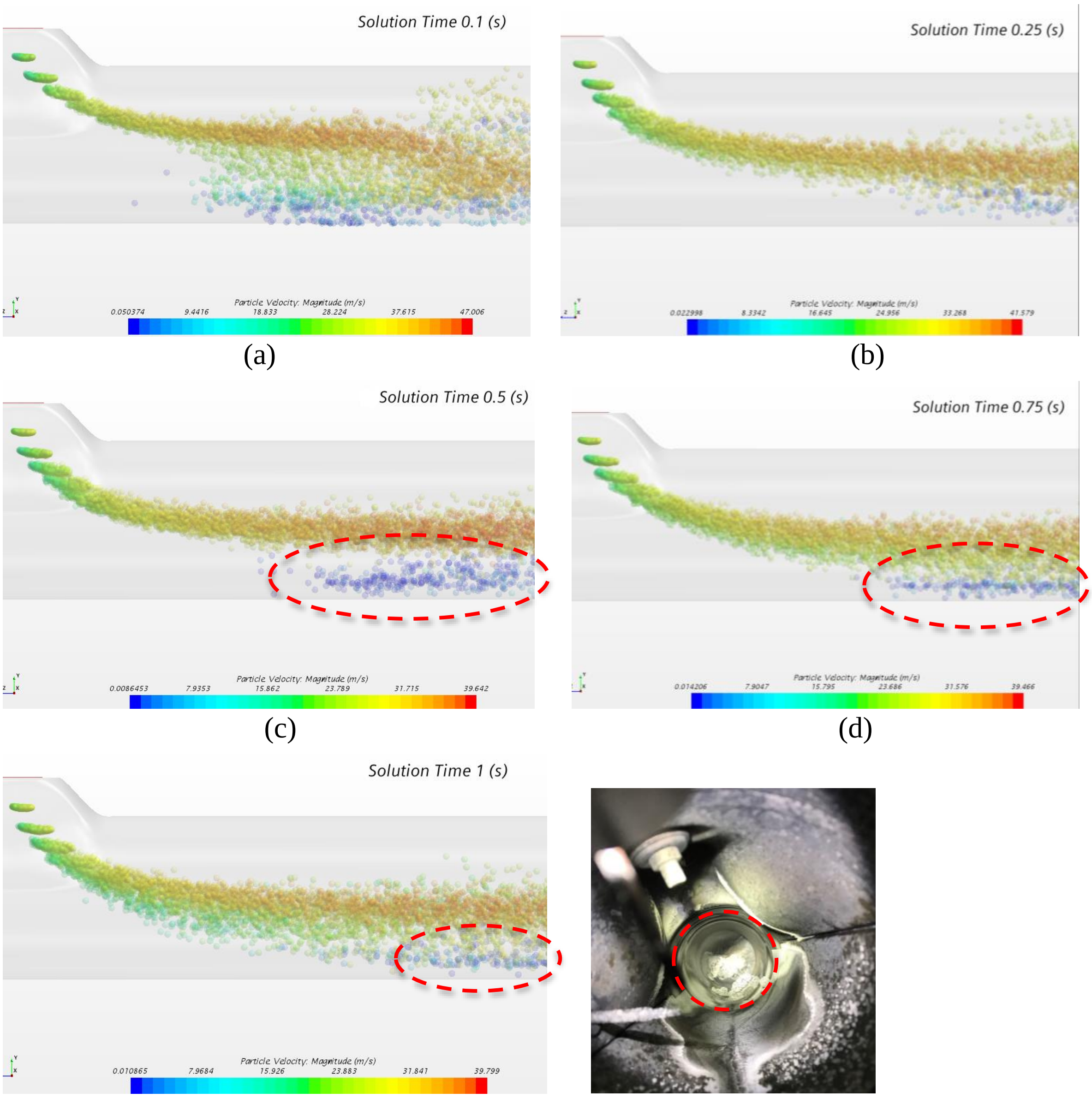


Figure 15: Test 1 Simulation images a, b, c, d, e respectively at 0.1, 0.25, 0.5, 0.75, 1,0 seconds

As it can be observed from the above Figure 15(a) at 0.1 seconds, the particle movement was so random. Since the flow has just started and would take some time to attain the required continuity and for the solution to converge. After 0.5 seconds in Figure 15(c) there are quite few blue particles with low velocities depicting that they are moving with slow speed on either bottom of the pipe or the sides. After the flow attains continuity, it can be observed that most of the spray has the high velocity and follows the exhaust through the pipe without causing any low velocity regions or stagnation along the walls.

As discussed with the test engineer at the Volvo Penta test basin - Razmjoo Narges, the present experiment scenario was explained as a clean pipe with level 0 crystals, A picture was captured relating to this case using a Biltema camera at the point of interest. Since the next consecutive experiment must be held, the time available for mantling and dismantling was short. The same can be seen in Figure 15(f) where the pipe is not consisting any white spots or lumps of urea crystals in it.

The same particle velocity scene is observed by designing the Test 18 simulation by changing the urea input to 0.32 g/s, wall temperature to 250, exhaust flow rates to 31.37 m/s. Then the following images shown below in Figure 16 are captured at the same times as the Test 1.



(a) (b)

(c) (d)

(e) (f)

Figure 16: Test 18 Simulation images a, b, c, d, e respectively at 0.1, 0.25, 0.5, 0.75, 1,0 seconds

As it can be observed from the above Figure 16, the same initial particle disturbance can be observed before the flow attains continuity. But comparing the results with Test 1, Test 18 shows the difference at around 0.5 and 0.75 seconds which can be observed in Figure 16 (c), Figure 16 (d) respectively (marked in dotted region for easy reference). The images depict that there is a slow stream of particles moving along the wall indicating that they are in contact to the wall due to a rapid decrease in the velocity, these conditions would be repeating for every frequency of spray resulting in a continuous contact with the wall surface and thus reducing the surface temperature of the wall are creating favorable conditions for the crystallization process.

As it can be seen in Figure 16(f) which was captured after the whole run of the experiment, the passage of the exhaust pipe is almost completely blocked by the crystals, the crystal level was estimated to be level 3 by the test engineer. Since it was hard to access and remove crystals from inside the muffler, the respective weights were not measured, and the muffler was considered not to be used for further experiments.

To further study this process the same Test 18 is repeated in Star-CCM+ but with a defining a section at 600 mm from the spray, to see the contact of particles as shown in the Figure 17 below

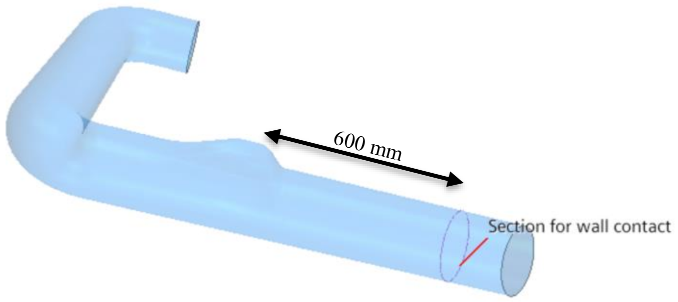


Figure 17: Image showing the section position for testing the particle contact

The following images below in Figure 18 depicts the same Test 18 results at the above-mentioned section defined to observe the contact region on the inner surface of the exhaust pipe by the spray particles.

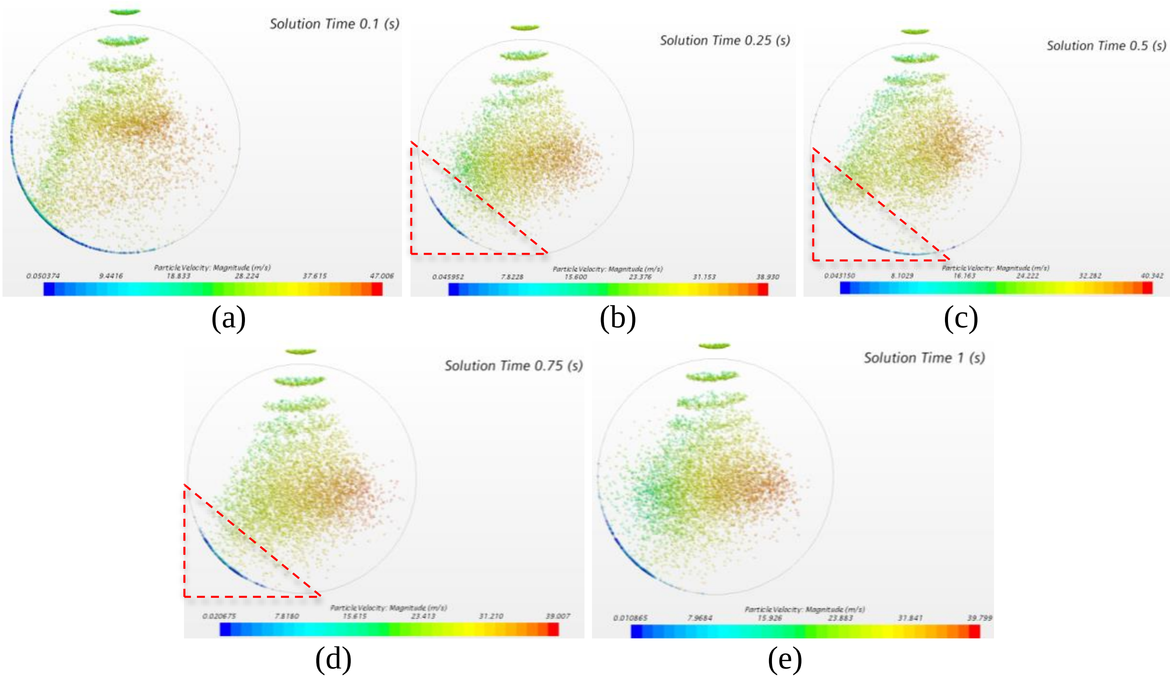


Figure 18: Sectional representation of Test 18 at 0.1, 0.25, 0.5, 0.75, 1,0 seconds

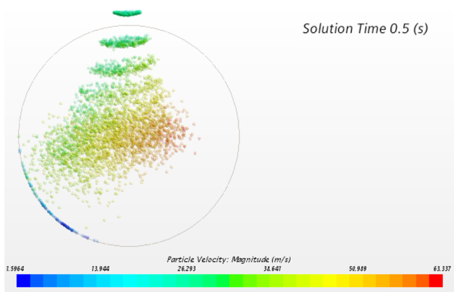
As it can be observed for every spray, there is a region of contact that's developing around 0.25 seconds and increasing during the mid-simulation at 0.5 seconds (marked in dotted region for easy reference). This is a continuous process that would occur for every single spray deflecting towards the wall with the Test 18 flow conditions. Confirming this during the thesis presentation at Volvo Penta, the engineers at the EATS department explained the happening of same phenomenon of spray wetting a single side, or the crystals starting to build up on one side of the wall proving the above simulated flow conditions.

To verify and support the above inference observed by the team, another experiment performed resulting in the level 3 crystallization has been chosen for simulation. But the inner iteration count has been reduced from 15 to 10 per timestep for reducing the time taken for the simulation. The below Table 3 indicates the data from Test 17.

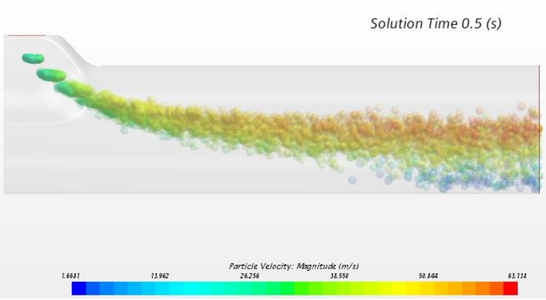
	Date	**Cycle**	**Hours**	**Fuel**	**Speed, Torque**	**Exhaust flow (kg/s)**	**velocity m/s**	**T_a Turb (C)**	**T_b_ SCR (C)**	**SensVal DPF Temp or calculated**
Test- 17	2019-11-30	D2(1800 rpm)P50	15	SD10	1800 rpm, 1475 Nm	0.56	50.50	301	306	309
	urea flow (g/s)	**Urea flow/Exhaust flow**	**Forced**	**Power (Kw)**	**Amount of crystals**	**Crystal Level**	**Weight of crystals (g)**	**Conversion**	**SO Nox**	**EO Nox**
	1	1.786	Yes	290	Much crystal in the SCR pipe	2 or 3	not removed	79.52	1.44	7.03

Table 3 : Table with data from Test -17

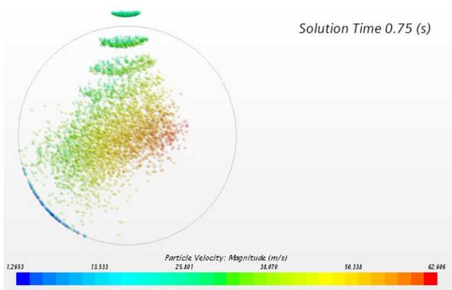
The same scenes of particle velocity at same time instants which are 0.5 and 0.75 seconds are designed for the output of simulation and similar results as the Test 17 were observed showing the wall wetting, slow moving particles that may lead to stagnation and cool down the region of contact over time. Just to limit the number of pictures only two-time frames of 0.5 and 0.75 seconds are represented below for reference.



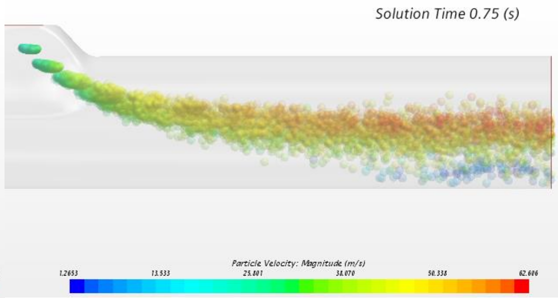
(a)



(b)



(c)



(d)

(e)

Figure 19: Test 17 Simulation images a, b and c, d at 0.5 and 0.75 seconds respectively

The Test 17 simulation is achieved by changing the urea input to 1 g/s, wall temperature to 300, exhaust flow rates to 50.50 m/s. As seen in the Figure 19 (e) the crystals are developed towards the right side of the pipe as seen from AdBlue injection point forward of exhaust pipe, which is the same phenomenon happening in the simulation. The assumptions made, and the properties defined show decent outcome through results without deviating much from the actual experimental results. Hence, the results were considered satisfactory by the EATS team and the simulation setup and supporting files were submitted to the team as a copy.

5. CONCLUSION

5.1 Variation of results:

Running the same simulation again and again would yield different results or different behavior of the particles but however the mass behavior pattern would almost be the same. It means that the cloud movement of the spray would be similar between simulations, but the individual particles may travel in different paths due to the simulation being implicit unsteady.

5.2 Parcel stream size Refinement:

A study on the Parcel size and Time consumed by simulation study been performed with conditions of Test 1 to decide the best possible trade of between parcel size and time taken. The below table

Parcel size	Time Taken by simulation
200	20 hours
250	28 hours
300	42 hours
400	62 hours
500	90 hours approx.

Table 4 : Parcel Size and Time Study

Depending on the available time and the processor capacities, different simulations are run on different CPU's with the parcel stream size set to 300. Refraining from using higher values of parcel size would result in the quality of the results but considering the time spent and the accuracy of results achieved. The parcel stream size of 300 seemed as a pretty good trade off.

Furthermore, for high values of urea dosing the parcel streams can be adjusted accordingly to not deviate from the accuracy of the results.

5.3 Mesh size Refinement:

To cope up with the availability of licenses and the computers in the Chalmers laboratory the process was made to speed up by minor refinements in the fine mesh sizing, the base size was increased from 4 mm to 5 mm and the base size near to the injector region was brought down to 1.5 mm. This showed a significant increase in the iteration speed. The timesteps were changed accordingly with the inner iterations set to 15 in most cases and 10 for the last few runs of simulations.

5.4 Relevance:

Summing up, the results achieved throw the models developed seemed accurate enough in predicting the flow without any anomalies. The results depicting the wall wetting and the most probable stagnation regions can be seen matching with the experimental data available showing that the results are trustable. However, the simulation can be furthermore simplified by removing the multicomponent liquid and replacing with a single liquid with the density of AdBlue solution, Also the wall temperature part can be removed if only the wall wetting property is the focus.

5.5 Steps for using the developed model:

The below mentioned steps can be followed with the provided simulation file for developing models for other 3D test models.

- Download the required 3D test piece model from CREO in any 3D file format.
- Import the same in either AutoCAD or Rhino.
  (Note: Any 3d modelling software can be use, respective commands may change).
- Delete all the other parts excluding the outer shell.
- Use the command 'JOIN' or 'UNION' to join all the shell surfaces.
- Extrude the ends of the 3D shell in required exhaust pipe shape using 'EXTRUDE'.
- Export the model to 'iges' or 'igs' file format.
- Open the simulation file provided as the base model with all the cores in parallel.
- In the Simulation tree, go to Geometry→3D CAD model→new→import→ igs file.
- Expand 3D CAD models, right click on imported model → new geometry part.
- Expand Parts →right click on Body →Repair surface →press ok
- Press execute →select all the edges on the inlet and outlet and press fill holes option.
- Press apply →expand operations →right click on Automated Mesh →Execute.
- Expand Regions →click on Boundaries and give inlet, outlet and the wall accordingly.
- Expand inlet → Physics values → Give the velocity magnitude of exhaust flow.
- Expand Injectors →Values → give the Axis and mass flow rates accordingly.
- Go to Inlet, Outlet and wall under regions and give the static temperature in physics.
- Go to Solvers → implicit unsteady →set the time step value to required.
- Go to Stopping criteria to change maximum inner iterations if necessary.
- Go to Stopping criteria to input the maximum physical time of simulation.
- Press Ctrl+T to run a single step and check if the residuals are converging.
- Press Ctrl+R to run the whole simulation.

5.6 Selection of post processing scenes:

Apart from the particle velocities different other parameters were tried and compared to show the best possible way to understand and explain the simulation results.

Parameters such as courant number to estimate the time step for better results and to check if it's in the limit (unity), heat transfer coefficient to understand the flow better but the changes in the heat transfer during one second of the simulation time were observed to be not satisfactory the same parameter of the heat transfer coefficient can be used if the simulation is repeated with number of spray cycles and much longer simulation time. Turbulent kinetic energy to understand the anomalies in the flow and to determine regions with high turbulence was used but this parameter has given the places of maximum and minimum energy points but would be hard to explain the results , mass fraction of H_2O to understand the evaporation effect which would happen as soon as spray enters the pipe making the post processing being observed only in few frames of output, velocity vectors to understand when the flow attains continuity, although if the comparison has to be made between different simulations using this parameters it would be confusing due to the arrows used as a representation of vector directions in the postprocessor and finally wall y+ which was used to determine and study the regime of boundary layer for better understanding of physics. After comparing thousands of images which are a resultant output from simulations the parameter particle velocity is chosen as the best possible way to predict the current phenomenon of crystallization as it gave the movement of the particle clouds throughout the regime of interest.

6. EXPERIMENTAL WORK

The prime motto of the experimental work is to build a flow-bench to visualize the flow-spray interactions thus reducing the costs required for running the test models in actual engine setup and load cycle. By this method the wall wetness and cold spots could be identified prior hand, hence giving a chance to improvise the model/spray setup.

The flow-bench can initially be setup as just a normal cold flow rig but can later be developed into a hot flow rig by adding heating elements and insulating components. By converting the experiment into a hot flow rig, concepts such as Liedenfrost effect, Evaporation, Angle of reflection of spray vs temperature can be observed and studied.

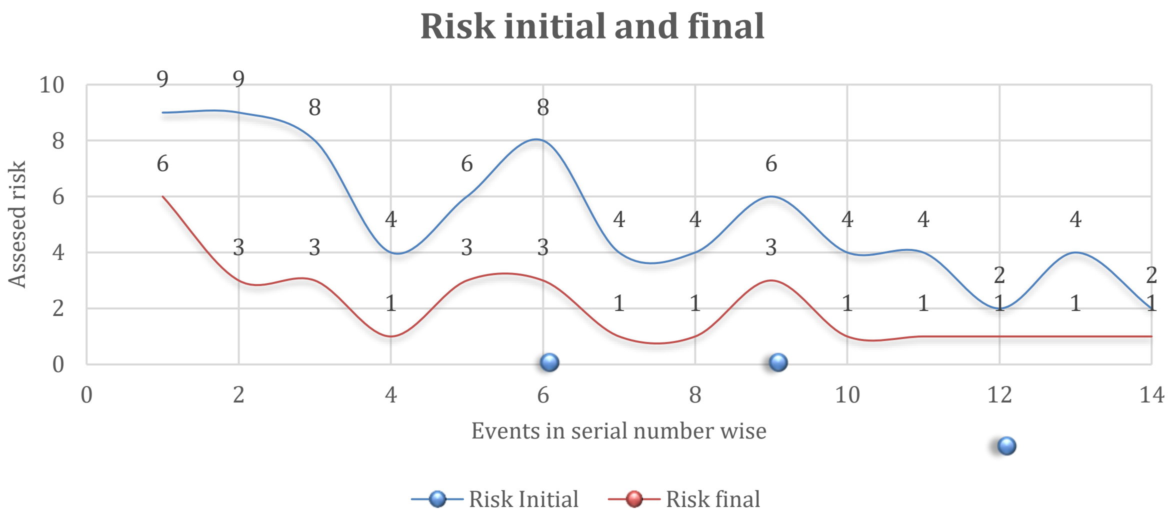
6.1 *Risk assessment:*

A detailed risk assessment was performed concurring with the Chalmers criterion, the risks assessed and the risk reduction actions in view according to the ERICPD are explained in detail in the Appendix -I. The below table provides the information of all the risks that may be involved for the experimental studies and the final remaining risk after the reduction action. The assessed risk in the table below is the product of probability and consequences of the risk identified.

Probability (P):	**Consequence (C):**	**Risk assessment**
4 Almost certain	4 Very serious	10 - 16 High risk
3 Likely	3 Serious	6 - 9 Medium risk
2 Less likely	2 Minor	1 - 5 Low risk
1 Unlikely	1 Insignificant	

Sl No.	**Risk (event)**	**Assessed risk**	**Remaining risk**
1	Risk of personal injury when lifting and moving objects	9	6
2	Risk of personal injury Due to extreme heat of experiment	9	3
3	Fire Hazard due to excess temperature	8	3
4	Risk of personal injury due to slipping or falling on uneven floor at the lab	4	1
5	Risk of personal injury due to defective tools	6	3
6	Electric Hazard	8	3
7	Ventilation and risk of suffocation	4	1
8	Release of steam/smoke	4	1
9	Inhaling Urea / ammonia vapors	6	3
10	Contact of Urea on skin	4	1
11	Space around the experiment	4	1
12	Spillage of chemicals/ AdBlue	2	1
13	Discharge of heated AdBlue	4	1
14	Storage of AdBlue and other equipment	2	1
		Ri_{total} = 79	**Rf_{total} = 29**

Table 5 : risk analysis for experimental studies.



Graph 1: risk analysis for experimental studies.

6.2 Design *of Phase I:*

A transparent model attached to an industrial grade air blower with a frequency modulator to stimulate the same quantitative flow as in the engine exhaust. Then the Spray behavior in the flow can be studied using a high-speed camera. The pictorial representation is shown in the below Figure 20.

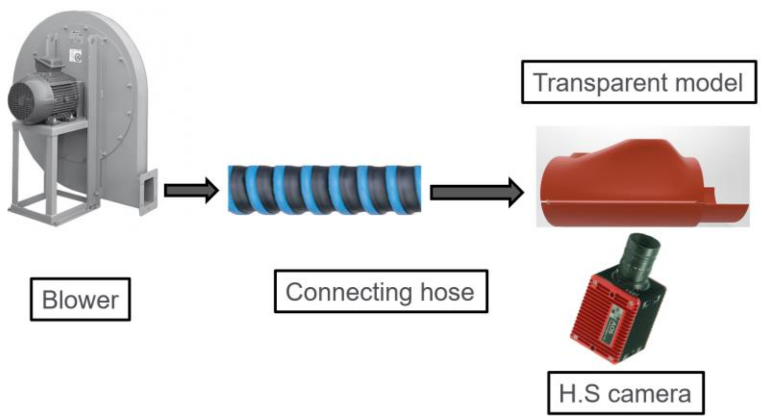


Figure 20: Pictorial representation of cold flow rig

The equipment details are listed below

5.2.1 Transparent models: Fabricated transparent models which are to be used for visualizing the spray from outside in phase I are enquired from different vendors like 'Prototal industries, Protech Nordic AB, Protolabs Sweden AB' etc. They have almost similar pricing of material and units. Since the Prototal has already signed an NDA (non-disclosure agreement) they were preferred for the confidentiality of the models. The initial enquired quotation is around SEK 24100. In which Fabricated model is around SEK 18500 and the Surface finish, lacquer, clearing varnish is around SEK 5600. The Tolerances of fabrication is mentioned to be SLA min ± 0.1 mm and ± 0,15 % of dimension.

5.2.2 Industrial grade blower (FC 801): Depending on the experiments carried out at Volvo Penta, the required flows are calculated. The maximum required flow is around 0.73 m^3/s or 0.726 kg/s and the minimum required flow for the experiments is 0.246 m^3/s or 0.304 kg/s. To develop the same flow as in exhaust, an industrial grade blower with frequency modulator is to be used. The same has been enquired from 'Industrial Fan Technology AB' with a primary quote of SEK 49700 (blower – SEK 33000, frequency modulator – SEK 16700). The blower consists of a single suction radial fan made of standard steel coated with water-based epoxy (RAL 7045, gray), Ferrari made and can withstand up to 200°C. It has a 2 pole, 3-phase, 50 Hz, 15 kW, 400V motor with a 3000 rpm and a IP-55 resistance. The Frequency modulator (FC 102) is 15 kW, 32 A and has a IP-55 resistance.

5.2.3 High Speed Camera (L-VIT 1000): For capturing minor details of the spray behavior a high-speed camera would be highly beneficial. A primary enquiry for the quote has been made with Quantum design and AOS Technologies, and the primary quote was given to be € 21,200 ≈ SEK 223412. The camera can go up to 1000 fps at a resolution of 1920x1080 and has a CMOS sensor. The Imaging Studio v4 SW software for easy integration. Light sensitivity is mentioned as ISO 8000 for mono and ISO 6000 for color. Exposure time is mentioned as global from 1/framing speed down to 2 microsec and a single charge can give 30 minutes of usage.

A secondary flexible camera for visualizing the internal surfaces can be purchased from Biltema. It has a Camera cable of 5 m length and a Camera head of 10 mm. The output resolution would be 1280x720 pixels @30fps or 1600x1200 pixels @12fps and is IP-67 water resistant. The price of a single unit is SEK 379.

The connecting hoses, lens, lighting required for the camera, flow meters and other supporting equipment can be considered as miscellaneous items.

6.3 Design of Phase II:

The main purpose of the heat flow rig is to see the similarity with the experimental test data that's in possession for IMO III D16 engine. The fabricated models used in phase-I will be here replaced by original steel test models. In addition to the setup in phase-I, heating elements will be used to heat the injection module to a required temperature. Engine experiment data available for IMO tier III D16 engine. Same temperature and flow conditions can be utilized to check the relevancy of the rig and to make conclusions. Caution should be taken in directing the urea vapors out of the test basin. The pictorial representation is shown in the below figure.

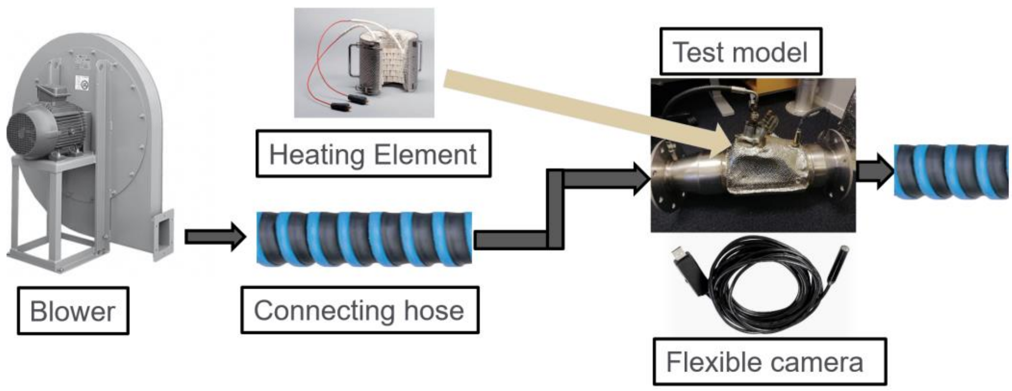


Figure 21: Pictorial representation of hot flow rig

The equipment details are listed below

6.3.1 Steel test models: Steel test pieces available at Volvo Penta can be used for the experiment. However, the hoses should be connected carefully with no possibility for the leaks of urea fumes.

6.3.2 Heating elements: To develop the same conditions of wall temperature as in exhaust, heating coils and insulations can be used. The same has been enquired from Weldotherm WTD with a primary quote of €5702.4 ≈ SEK 60170. As per the discussion with the Weldotherm, there may be a requirement of the following to maintain the required surface temperatures on the injection module. One each inverter heating unit (WR10.5) with cables, 15m long which costs EUR 4.250,00, two each wraparound heater for 128mm pipe 60V, 2.7kW, 45A costing EUR 301,70 each, one each thermocouple welding unit (TP-2N) which is EUR 750,00 for a unit and one each thermocouple wire 2 x 0.5mm, 100m which is EUR 99,00 each.

The insulating material, electrical wires, thermometers and other supporting equipment are considered as miscellaneous and generalized electrical and electronics.

6.4 Budget and Bill of materials:

The Table 6 below gives an estimation of costs that may be involved in performing the experiments. Of all the highspeed camera is the expensive and the amount quoted below is excluding the lens and lightening needed. The miscellaneous items such as bolts, screws, pipes, AdBlue solution etc. are estimated to a number and are not exact. The electrical consumption, wires and electronics required are in the Elec and Electronics section. An overall total of around SEK 412190 is estimated as first guesstimate. However, if the HS camera is removed and only a single transparent model used then the guesstimate would come down to a total of around SEK 155000.

Details		**Cost estimation**		
Sl No:	Component	Cost (SEK) per unit	Quantity	Sum
1	Protech Transperant printed model	24,100 kr	2 Nos	48,200 kr
2	High Speed Camera excl Lens	2,33,200 kr	1 Nos	2,33,200 kr
3	Biltema flexible camera	379 kr	1 Nos	379 kr
4	Heating elements	62,711 kr	1 Nos	62,711 kr
5	Fan/Blower	49,700 kr	1 Nos	49,700 kr
6	Misc	15,000 kr	1 Nos	15,000 kr
7	Elec & Electronics	3,000 kr	1 Nos	3,000 kr
			Total :	4,12,190 kr
			Total excl HS camera and only one model :	1,54,890 kr

Table 6: Cost estimation for the Experimental Studies

Depending on the funds available at the time of experiments, a decision can be made on purchasing.

7. Future work

- The speed up method which was proposed by Siemens using the method of co-simulation, speeding up the process by around a factor of 20 can be studied and implemented for this study in simulating the computational AdBlue spray and the liquid film.
- Running the simulations on Cluster with all the settings set to maximum including a good number of parcel size and with a finer mesh would give better results.
- Adjusting the material properties further accurate by feeding more polynomial verses temperature values for both the multi component gas and multicomponent liquid modules in the software.
- Investigating the other tests with the data available and correlating the exhaust flow rates, urea dosing values and at which time of the second the spray would be easy to deflect would be a good way to predict the crystallization, if the same test piece is used.
- Modelling the same simulations for different other test pieces for comparison.
- Investigating on the availability of other transparent 3-D printed or molded test pieces from other possible vendors.

Appendix

Risk Analysis for Experimental methods:

Probability	Consequence (C):	Risk assessment	ERICPD
4 Almost	4 Very serious	10 - 16 High risk	E = Eliminate
3 Likely	3 Serious	6 - 9 Medium risk	R = Reduce
2 Less likely	2 Minor	1 - 5 Low risk	I = Isolate
1 Unlikely	1 Insignificant		C = Control
			P = Personal protective
			D = Discipline

Risk assessment performed/updated by:	Naga Siva Sai Tarun Madisetty
Assessed area:	WorkPlace Volvo Penta
Date:	2/20/2020

Sl No.	Risk (event)	Risk description (Cause)	Consequence	Comments and existing barriers	P	C	Assessed risk	Risk reduction action as per (ERICPD).	Responsible	Completion date	P	C	Remaining risk	Result / finishing conclusion, or description of future action. References (role, procedure, etc.).
1	*Risk of personal injury when lifting and moving objects*	*Careless handling of equipment can lead to minor to major injuries*	*Can cause a delay and flexibility in work due to recovery or pain*	*All the required equipments are not available at the location and there is always a need to mantle and dismantle some equipment and requires usage of tools*	3	3	9	*Taking precautions like putting on gloves and safety equipments.detailed study of operation before practical usage. Help from recomended personal for required jobs.*	*Tarun; Thesis student*	*12/2/2020*	2	3	6	
2	*Risk of personal injury Due to extreme heat of experiment*	*The test piece will not be insulated so contact with the test piece or other heating elements would lead to severe injury*	*severe burning would occur if a person gets in contact with the equipment while its hot.*	*Objective of experiment as of now requires usage of heat.*	3	3	9	*Educating all whoever is visiting the experiment about the temperature of the equipment and using thermal insulated safety equipment in order to operate the heated elements*	*Tarun; Thesis student*	-	1	3	3	
3	Fire Hazard due to excess temperature	Due to high temperatures, flammable materials that come in contact would would ignite and be a fire hazard	Fire in the workplace	*Objective of experiment as of now requires usage of heat.*	2	4	8	*Educating all whoever is visiting the experiment about the temperature of the equipment and removing elements such as papers, cotton and easily flammable materials from the place of experiment*	*Tarun; Thesis student*	-	1	3	3	
4	Risk of personal injury due to slipping or falling on uneven floor at the lab	slippery and uneven floor can cause unbalance while walking and may lead to accidents	injuries ranging from minor to major	*the workplace for the experiment is in the basement and is fixed.*	2	2	4	*checking if the floor is slippery or presence of any liquids on floor. Making floor to be even in first hand.*	*Tarun; Thesis student*	-	1	1	1	
5	Risk of personal injury due to defective tools	Defective tools may break or loose contact from equipment and lead to injury	*Can cause a delay and flexibility in work due to recovery or pain*	*There will be a certain requirement of tools for fixing and dismantling of equipment*	2	3	6	*Making sure that the*	*Tarun; Thesis student*	-	1	3	3	
6	Electric Hazard	Electric heating and usage of blowers requires electric connection, which can short circuit or deliver electric shock	damage of equipment, fire and electric hazaard	*electricity usage can be minimized but not eradicated.*	2	4	8	*loose and improper connections should be rectified and experienced electrician should be consulted for the equipment connections with the outlet. Euipment should be disconnected from power when not in use.*	*Tarun; Thesis student*	-	1	3	3	
7	Ventilation and risk of suffocation	heated equipment radiate heat increasing the ambient temperature, leading to discomfort in breathing if sufficient air supply is not provided.	discomfort during operation, health issues.	*objective iof experiment as of now requires usage of heat.*	2	2	4	*proper ventilation in the lab is checked. The main door will be kept open during the experiment.*	*Tarun; Thesis student*	-	1	1	1	
8	Release of steam/smoke	heating of adblue and water solution may release steam/smoke if the exhaust is not adequate	raising of alarms and feeling of discomfort.	*objective iof experiment as of now requires usage of heat.*	2	2	4	*proper exhausting system in the lab is checked. The main door will be kept open during the experiment.*	*Tarun; Thesis student*	-	1	1	1	
9	Inhaling Urea / ammonia vapours	heating of adblue would release fumes if not well contained	beathing and exposure to these fumes would lead to health issues	*Adblue is a solution to be tested for the crystallization.*	2	3	6	*proper exhausting system in the lab is checked. The main door will be kept open during the experiment.*	*Tarun; Thesis student*	-	1	3	3	
10	Contact of Urea on skin	Prolonged contact with the adblue solution would lead to allergies and rashes on skin	skin becomes sensitive and can cause inflammation	*Adblue is a solution to be tested for the crystallization.*	2	2	4	*Using proper clothing and gloves when ever the contact with adblue is being made.*	*Tarun; Thesis student*	-	1	1	1	
11	Space around the experiment	cramped space can create improper activity and difficulty to escape an accident.	can delay the work or decrease the efficiency of work	*the alloted space cannot be changed*	2	2	4	*moving equipment present inside the lab to provide sufficient space for ease of experiment.*	*Tarun; Thesis student*	-	1	1	1	
12	Spillage of chemicals/ AdBlue	Urea solution can be spilled while transferring or working with the injectors	can cause stains or rashes on skin or can make the floor slippery	*Adblue is a solution to be tested for the crystallization.*	2	1	2	*Care should be taken to prevent spills and necessary cleaning action should be taken asap*	*Tarun; Thesis student*	-	1	1	1	
13	Discharge of heated adblue	improper discharge may block the pipes and equipment as it crystallises .	may create back pressure, change the internal flow for later experiment. Contamination of air in lab.	*Adblue is a solution to be tested for the crystallization.*	2	2	4	*the exhaust line should be planned accurate.*	*Tarun; Thesis student*	-	1	1	1	
14	Storage of Adblue and other equiment	Improper storage may lead to evaporation and crystallization.	the adblue and equipment cannot be further used.	*Adblue is a solution to be tested for the crystallization.*	2	1	2	*the storage should be airtight and all the pipes should be cleaned and run back before stopping the experiment (no solution in lines)*	*Tarun; Thesis student*	-	1	1	1	
					Ri_{total} =		74				Rf_{total} =		29	

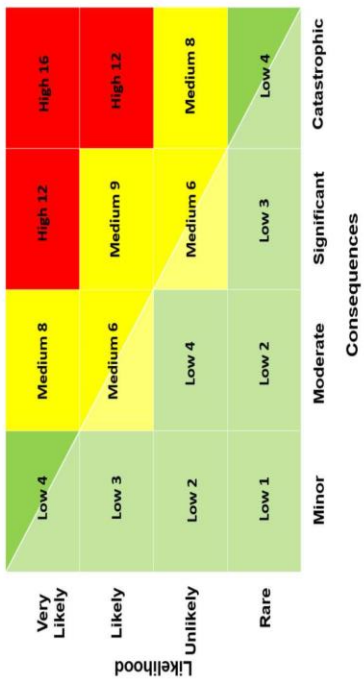
Figure i: Risk analysis for experimental methods (1)

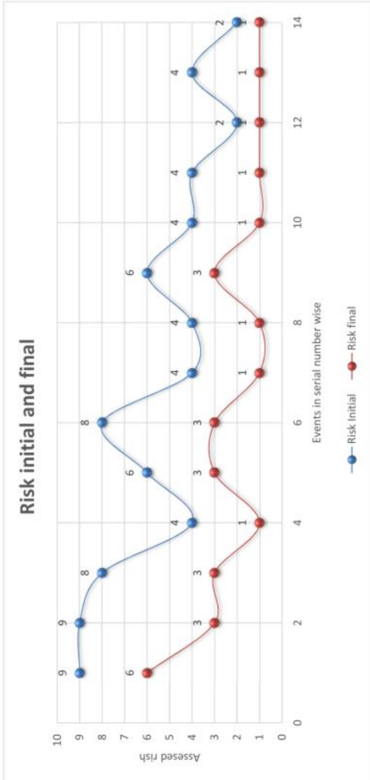
Risk Analysis for Experimental methods – Chalmers model:

Chalmers Risk Assesment model

Definition	Probability: Dimension	Level	Definition	Consequence: Working environment	Level	Consequence: Security	Level	Consequence: Environment	Level
Almost certain	The event is expected to occur under	4	**Very serious**	• Accident that results in death	4	• Extensive destruction/damage to buildings,	4	• Long-term or permanent very serious impact on	4
Likely	The event is likely to occur under most	3	**Serious**	• Significant/serious personal injury	3	• Damage to buildings, premises and	3	• Medium or long-term serious impact on a	3
Less likely	The event could occur on a few isolated	2	**Minor**	• Minor personal injury that requires	2	• Individual buildings or laboratories are	2	• Short-term serious impact on the external	2
Unlikely	The event could only occur under	1	**Insignificant**	• Minor personal injuries that do not	1	• Individual buildings and laboratories require	1	• Incidents or near-accidents with no or	1

[*] The term financial losses is given a broad definition, an actual and realised cost, an estimated cost, a loss of revenue, a loss of efficiency with known effect, etc





Risk value

Low risk	1 - 5
Medium risk	6 - 9
High risk	10 - 16

Risk value is the product of probability x consequence

Figure ii: Risk analysis for experimental methods (2)

Urea crystal levels inside the exhaust pipe:

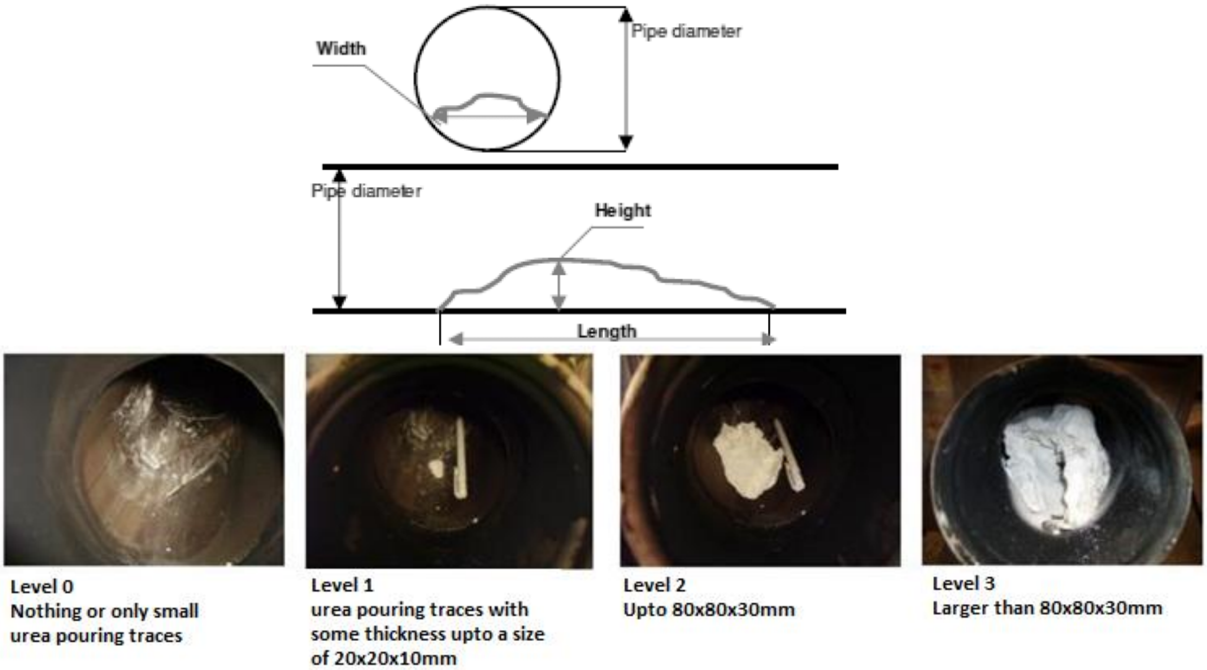


Figure iii: Levels of Urea crystals and dimensions of crystals

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