A study on post impingement effects of urea-water solution spray on the heated wall of automotive SCR systems

G M H Shahariar, M K A Wardana and O T Lim*
School of Mechanical Engineering, University of Ulsan, Ulsan, 680-749, Korea

E-mail: otlim@ulsan.ac.kr

Abstract. The post impingement effects of urea-water solution spray on the heated wall of automotive SCR systems was numerically investigated in a constant volume chamber using STAR CCM+ CFD code. The turbulence flow was modelled by realizable k-ε two-layer model together with standard wall function and all y+ treatment was applied along with two-layer approach. The Eulerian-Lagrangian approach was used for the modelling of multi phase flow. Urea water solution (UWS) was injected onto the heated wall for the wall temperature of 338, 413, 473, 503 & 573 K. Spray development after impinging on the heated wall was visualized and measured. Droplet size distribution and droplet evaporation rates were also measured, which are vital parameters for the system performance but still not well researched. Specially developed user defined functions (UDF) are implemented to simulate the desired conditions and parameters. The investigation reveals that wall temperature has a great impact on spray development after impingement, droplet size distribution and evaporation. Increasing the wall temperature leads to longer spray front projection length, smaller droplet size and faster droplet evaporation which are preconditions for urea crystallization reduction. The numerical model and parameters are validated comparing with experimental data.

1. Introduction

In order to meet the progressive compact emission legislation, such as Euro 6, engine manufacturers are being forced to install exhaust after treatment devices to meet the raising challenge. The selective catalytic reduction (SCR) is the most felicitated automotive exhaust gas after treatment solution for nitrogen oxides (NOx) emissions reduction which is capable of meeting most of the emission standards [1]. Ammonia (NH₃) gas reacts with the flowing exhaust gas into the SCR device and converts the NOx element into nitrogen (N₂) gas and water (H₂O) [2]. Though NH₃ is a noxious chemical component and harmful for human heath, urea is used as the precursor of NH₃ gas, which can be easily handled and transported [3]. Urea-water solution (32.5% urea by weight) known as Ad-Blue is injected into the exhaust gas stream by means of an injector, and then urea is decomposed to ammonia (NH₃) gas [4]. Urea decomposition is very slow process and catalyst is required, as a result isocyanic acid reacts with undecomposed urea and produces complex polymers such as melamine,
biuret, ammeline, triuret, cyanuric acid and ammelide [5]. According to the study of Xu et al. [6] solid deposits are formed below 300° C temperature in SCR system. These by-products (urea deposits) are accumulated on the injector tip, exhaust pipe wall, catalyst surface, mixing element and reduce the catalyst activity, increase engine backpressure, thus lower the NOx conversion rate and gradually make the system ineffective. When the exhaust temperature is more than 350° C, the deposits are vaporized gradually, but thermal decomposition of deposits are very slow, the rate is about 2 mg/min at 873 K temperature [7]. So optimization of the UWS spray is the most feasible way to minimize deposit formation.

For acquiring this specific purpose Computational fluid dynamics (CFD) analysis can be the effective tool for the designers. Application of automatic meshing approach can be operative here to assure the maximum possible prediction accuracy within a short time frame. In the purpose of urea-SCR simulation various modelling approaches such as ammonia homogenization [8], deposit formation are established. Spray-wall interaction is the most complicated and significant phenomena, that is modelled by Bai-Gosman [9] and others. For the proper understanding of UWS droplet impingement process and mechanisms underlying behind this, an intensive investigation is required in a constant volume environment, where only spray wall impingement take place. This paper presents a three dimensional numerical modelling and analysis of UWS spray wall impingement to investigate the post impingement effects on the heated wall of SCR system using STAR CCM+. The numerical simulation measured the axial and radial distance of UWS spray after impinging on the heated wall. The numerical visualization and measurements are compared and validated with the experimental results. Moreover, the simulation estimated two crucial parameters; UWS droplet size distribution and UWS droplet evaporation rate after the start of injection using the specially developed user defined functions (UDF). A detailed analysis was carried out to gain a deep understanding about the post impingement effects and the causes beyond deposit formation in SCR systems.

2. Simulation conditions

The urea-water solution (UWS) known as Ad-blue was sprayed on the heated wall by means of a single hole pressure swirl injector in a non-reacting environment.

| Table 1. Spray simulation case setup and conditions. |
|-----------------------------------------------|
| **Parameter** | **Value** |
| Injected liquid | UWS (32.5% wt. urea) |
| Injection duration | 10 ms |
| Height from the wall, h | 30 mm |
| Injection pressure, P_{inj} | 0.47 Mpa |
| Injector nozzle hole diameter | 0.55 mm |
| Injection angle, θ | 90° |
| Half cone angle, Φ | 29° |
| Wall temperature, Tw | 338, 413, 473, 503, 573 K |

3. Numerical modelling

The interaction between each particle or parcel and with the continuous phase are modelled in Eulerian-Lagrangian approach using the incompressible and unsteady Reynolds averaged...
Navier-Stokes (RANS) equations for energy, mass, momentum and species. The realizable k-\varepsilon model is applied for the modelling of the turbulent flow because it has improved ability over standard k-\varepsilon model in case of turbulence quantities estimation. The primary spray atomization for the thin liquid sheet produced at the nozzle tip, created by the pressure swirl atomizer is modelled by Linearized Instability Sheet Atomization (LISA) model [10]. For modelling the droplet size distribution an empirical function known as Rosin-Rammler distribution is used [11]. The collision between the droplets are estimated by the NTC (No Time Counter) collision detection algorithm [12]. The atomized droplet trajectories are estimated by Newton’s second low of motion that states the momentum rate change is equal to the summation of forces acting on the particle. The quasi steady evaporation rate of each component is described as

\[ m_{\text{ev}} = -\zeta g^* A_s \ln(1 + B) \]  

Here, B denotes Spalding transfer number, as denotes the surface area of droplet, g* denotes the mass transfer conductance, \( \zeta \) represents the fractional mass transfer rate. The commercial simulation software STAR CCM+ is used for solving the governing equations. The second order upwind scheme is executed for multiphase simulations, because it has better accuracy than the first order scheme. In droplet wall interaction modelling Leidenfrost temperature effect is implemented using a specially developed user defined function (UDF) subroutine. Two more UDF are implemented to solve the droplet size distribution and droplet evaporation. All y+ treatment was applied along with two layer approach. The residuals for energy, turbulent kinetic energy, turbulent dissipation rate, momentum, temperature, continuity and each species were inspected until stabilization to trace the convergence. In this work, automatic meshing technique was used with a base size of 5 mm volume mesh type. Two prism layers with 2 mm thickness were used for resolving the near wall region flow accurately. Sensitivity analysis was done for mesh base size 4 mm and 3 prism layers and the other settings were remained same.

4. Results and discussion

During the simulation study three crucial parameters (spray development after impingement, droplet SMD and droplet evaporation) have been investigated and analysed to reveal the post wall impingement effects in diesel SCR system.

4.1. UWS spray wall impingement at low wall temperature (338 K)

UWS spray development after impinging on the heated wall for a wall temperature 338 K is seen in figure 1. Figure 2 illustrates the comparison of the numerical and experimental UWS spray visualization of UWS spray wall impingement for a wall temperature 338 K and for three separate time intervals; t = 5, 8 & 10 ms after the start of injection. The droplets of the numerical images are coloured based on their velocities. The acting wall temperature is lower than the boiling point temperature of water. After impingement UWS spray droplets are adhered on the wall surface and urea deposits are formed, if the temperature of the wall is lower than 450 K. The hollow cone spray produced by the current numerical simulation is analogous with the experimental visualization. The UWS spray projected radially after impacting on the heated wall, which is clearly seen in current simulation and experimental visualization. A detailed look onto the measurements of axial and radial distance of UWS spray after impinging on the heated wall is presented in figure 3. Axial distance travelled by the UWS spray after impinging on the heated wall is in good agreement at all the three
analysis; radial projection distance measurements are harmonious with the experiment but Abu-Ramadan simulation measurements are deviated.

4.2. UWS spray wall impingement at high wall temperature (573 K)

Figure 4 shows the spray impingement phenomena after impinging on the heated wall for the wall temperature 573 K. Figure 5 shows the comparison of the numerical and experimental UWS spray visualization for three separate time frames; \( t = 5, 8 \) &\( 10 \) ms after the start of injection. A little deviation stands between the experimental and current numerical visualization. The splashed/rebounded droplets in the current simulation are analogous with the experiment. In the experimental images vaporized wavy region can be seen, but Lagrangian particle tracking unable to display those phenomena. In the current simulation study, the spray development area seems smaller than the experiment, this is because the evaporated droplets are not shown in simulation visualization.

Figure 6 shows the quantitative comparison of the axial and radial distances of UWS spray after impinging on the heated wall. The current simulation underestimates the axial and radial distances in comparison with the experiment, after impinging on the heated wall. This is because the simulation visualizations are not showing the evaporated droplets, hence the axial and radial distances reduced, but the current simulation results are identical with the experimental measurements.
4.3. Droplet size distribution for different wall temperature

Figure 7 presents the sauter mean diameter (SMD) of the UWS droplets after the start of injection, for wall temperature 338, 413, 473, 503 & 573 K. During the UWS spray impinging on the heated wall, small size droplets evaporate faster that leads to form higher active elements during the same time, therefore the exhaust gas and SCR reductant mixes uniformly, thus deposit formation is reduced. Simulation studies reveal that the droplet SMD is almost same for the wall temperature 338, 413, 473 and 503 K, so urea solid deposit formation risk is still high until the wall temperature 503 K. The SMD is stabilized quickly for high wall temperature (573 K). The maximum value is 98 µm for 338 K wall temperature and 51 µm for 573 K wall temperature, which is about half of the first case. Shorter liquid phase exhibit period is better for faster droplet evaporation; the value is 1.3 ms for 338 K wall temperature and 0.3 ms for 573 K wall temperature.

4.4. Evaporation behavior of UWS

Rapid evaporation of UWS is recommended for the reduction of urea deposits formation. Figure 8 shows the evaporation rates of UWS for wall temperature 338, 413, 473, 503 & 573 K. It is seen that, the UWS droplets evaporation rate increases gradually for lower wall temperature to higher wall temperature and it goes to the peak for 573 K wall temperature. The highest value is 1.65e-6 kg for 573 K wall temperature and 4.02e-7 kg for 338 K wall temperature. Therefore, high temperature operation is advantageous for the reduction of deposit formation.

5. Conclusion

In order to address concerns about the effects of wall impingement of UWS on the heated wall of SCR systems, a numerical study has been conducted using STAR CCM+ CFD code. The spray wall impingement, droplet size distribution and droplet evaporation rates are analysed and the effects of wall impingement on urea deposits formation are investigated under different ambient conditions. The simulation results are compared with Birkhold experiment [13] and Abu-Ramadan et al. simulation [14]. Following conclusions are drawn from the study.

(1) The wall temperature significantly influences the development of UWS spray after impinging on the heated wall. The development of spray front (radial projection) is larger at high wall temperature...
and axial length is smaller i.e larger spray distribution area, which is better for efficient mixing and evaporation thus lower urea deposits formation and vice versa for low wall temperature. 

(2) The predicted SMD is rather small in high wall temperature and small droplets evaporated completely.

(3) The evaporation rate is very slow at low wall temperature in comparison to high wall temperature, this is because the simulation is predicted much higher size droplets and lower radial projection distance at low wall temperature operation.

Acknowledgments
This research was financially supported by the Global-Top Project of Korea Ministry of Environment (2016001420002, Development of the PM-NOx purifying system and the core technology).

6. References
[1] Johnson T. 2016 SAE Int. J. Engines 9(2):1258-1275
[2] Selective catalytic reduction. (Online), 2009 (cited 2017-02-10), Available from: http://www.dieselnet.com/tech/cat_scr.php
[3] Salib R. and Keeth R. 2003 Proce. of Mega Symposium
[4] Fritz, A. and Pitchon V. 1997 Appl.Catalysis B: Environ. 13(1), 1-25
[5] Birkhold F. Meingast U. Wassermann P. and Deutschmann, O. 2006 SAE Tech. Paper 2006-01-0643
[6] Xu L. Watkins W. Snow R. Graham G. et al. 2007 SAE Tech. Paper 2007-01-1582
[7] Way P. Viswanathan K. Preethi P. Gilb A. et al. 2009 SAE Tech. Paper 2009-01-0633
[8] Fischer S. Bitto R. Lauer T. Krenn C. et al. 2012 SAE Int. J. Engines 5(3):1443-1458
[9] Bai C. and Gosman A. 1995 SAE Tech. Paper 950283
[10] Senecal P.K. Richards K.J. Pomraning E. Yang T. Dai M.Z. McDavid R.M. Patterson M.A., Hou, S. and Shethaji T. 2007. SAE Tech. Paper 2007-01-0159
[11] STAR CCM+ version 11.04 Theory Guide, 2016
[12] Schmidt D.P. and Rutland C.J. 2000. J Comp. Phy.
[13] Birkhold F. 2007 Untersuchung der Einspritzung von Harnstoffwasserlösung. Shaker
[14] Abu-Ramadan E. Saha K. and Li X. 2012 SAE Tech. Paper 2012-01-1301