

# Prediction of Spray Behavior in Injected by Urea SCR Injector and the Reaction Products

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## ABSTRACT

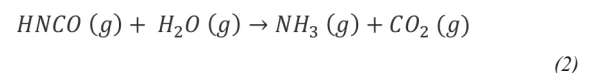
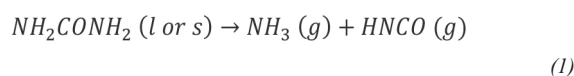
In the urea SCR system, urea solution is injected by injector installed in the front stage of the SCR catalyst, and NOx can be purified on the SCR catalyst by using NH<sub>3</sub> generated by the chemical reaction of urea. NH<sub>3</sub> is produced by thermolysis of urea and hydrolysis of isocyanic acid after evaporation of water in the urea solution. But, biuret and cyanuric acid which may cause deposit are sometimes generated by the chemical reactions without generating NH<sub>3</sub>. Spray behavior and chemical reaction of urea solution injected into the tail-pipe are complicated. The purpose of this study is to reveal the spray behavior and NH<sub>3</sub> generation process in the tail-pipe, and to construct the model capable of predicting those accurately. In this report, the impingement spray behavior is clarified by scattered light method in high temperature flow field. Liquid film adhering to the wall and deposit generated after evaporation of water from the liquid film are photographed by the digital camera. NH<sub>3</sub> concentration is measured at 13 points of the cross section of the tail-pipe by FTIR, and NH<sub>3</sub> concentration distribution is calculated. From the experiment, the influences of gas temperature on droplets scattering after wall impingement and impingement conditions on NH<sub>3</sub> concentration distribution are clarified. It is suggested that the deposit after evaporation of liquid film may be an intermediate product such as biuret or cyanuric acid. Also, by comparing and verifying the results of calculation using CFD software FIRE v2014.2 and the experimental results, the phenomenon influencing the prediction accuracy of the NH<sub>3</sub> concentration distribution is clarified. Factors influencing the prediction accuracy of calculation are atomization characteristics after wall impingement for NH<sub>3</sub> concentration, gas flow in the tail-pipe for NH<sub>3</sub> concentration distribution and liquid film generation due to the decrease of the plate temperature for NH<sub>3</sub> generation process.

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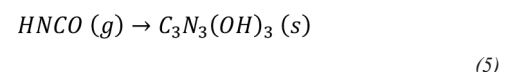
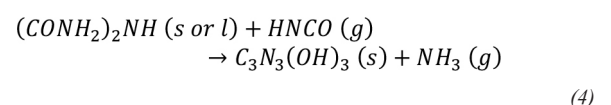
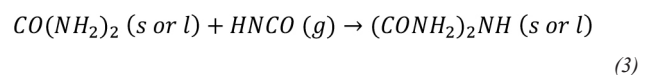
## INTRODUCTION

In order to cope with the exhaust gas regulation, introduction of a post-treatment device is indispensable [1]. Urea selective catalytic reduction (SCR) system is used to reduce NOx contained in exhaust gas from diesel engines. In the urea SCR system, urea water is injected by an injector installed in the front stage of the SCR catalyst, and NOx can be purified on the SCR catalyst by using ammonia (NH<sub>3</sub>) generated by the chemical reaction of urea [2].

As shown in [Figure 1](#), the wall impingement spray mechanism injected into the tail-pipe can be classified into free spray region, impingement spray region, evaporation of liquid film and separation droplets region, and urea solution dispersion region. Then, after water in the urea solution evaporates in each region, NH<sub>3</sub> is generated from the urea by a chemical reaction.



[Equation 1](#) represents thermolysis of urea, and [equation 2](#) shows hydrolysis of isocyanic acid generated by thermolysis of urea. But, biuret and cyanuric acid which may cause deposit are sometimes generated by the chemical reactions shown in [equation 3](#), [4](#) and [5](#) without generating NH<sub>3</sub> [3].





duration  $t_{inj}$  was 95.4ms. In the case of photography of liquid film and deposit and measurement of  $\text{NH}_3$  concentration distribution, the injection period  $f$  was 1Hz and the number of injections was 60. The gas temperature  $T_g$  to be introduced into the visualization tail-pipe was 250, 300 and 350°C. The gas velocity  $V_g$  in the pipe of  $\phi 10$  was 10m/sec. The distance  $H$  from the nozzle tip to the plate was 100mm. The plate angle  $\theta_p$  was 0° and 45°, and the injection angle  $\theta_s$  was 45° and 90°. The condition that the plate angle is 0° and the injection angle is 90° is defined as condition A, the condition that the plate angle is 0° and the injection angle is 45° is defined as condition B, the condition that the plate angle is 45° and the injection angle is 45° is defined as condition C and the condition that the plate angle is 45° and the injection angle is 90° is defined as condition D.

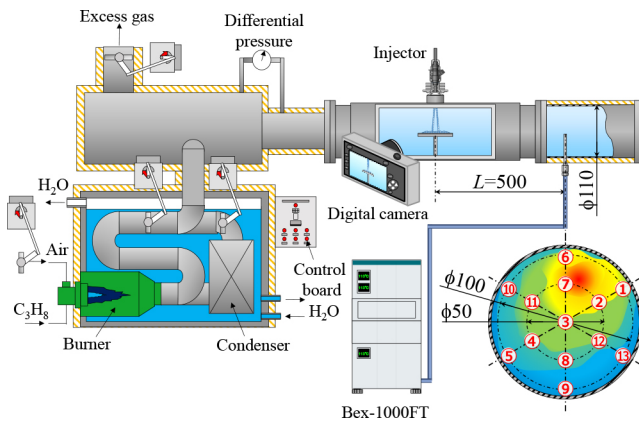


Figure 4. Experimental setup for  $\text{NH}_3$  measurement

## EXPERIMENTAL RESULT AND DISCUSSIONS

### Photography of the Impingement Spray

Figure 5 shows the results of scattered light method at the impingement spray. The figure is results when  $t/t_{inj}$  is 1.0.  $t$  is photographing timing. In all gas temperature conditions, the scattered light luminance of the droplet after impinging on the plate is higher than the free spray. Therefore, it can be seen that the atomization after the impingement is promoting. As the gas temperature rises, the Reynolds number decreases and the gas turbulence is restrained. As a result, it can be seen that the nonuniformity of the droplet distribution decreases as the gas temperature rises. Furthermore, the nonuniformity of the droplet distribution after impinging on the plate is decreased. The impingement spray behavior can be classified by boiling region determined by the superheat degree which is the difference between the saturation temperature of droplet and the plate temperature [4]. Since the plate temperature is equal to the gas temperature, it can be classified into a transition boiling region at gas temperature of 250°C and 300°C, and a film boiling region at gas temperature of 350°C [5]. In the film boiling region, since the droplet floats without adhering to the plate, the frictional resistance between plate surface and droplet is reduced. Therefore, it is considered that the nonuniformity of the droplet distribution was decreased by scattering to slide on the plate. In the condition C, since urea solution is injected from the upper direction, the droplet after impingement bounces backward against the gas flow and scatters from the lower side of the plate. Then, the droplet influenced by the gas flow are

pushed back and scatter from the upper side of the plate. As the gas temperature rises, droplets scattering from the lower part of the plate increase. This is meant to be the influence due to the difference in the boiling region. In the film boiling region where the gas temperature is 350°C, as it scatters to slide on the plate after the impingement, the droplets are hardly pushed back to the gas flow, and the number of droplets scattered from the lower side of the plate increases.

Figure 6 shows the spray tip penetration in the flow direction. The spray tip penetration is defined as the longest distance from spray impingement point to the droplet scattered in flow direction. Additional experiments were carried out in the condition that the gas temperature was 200°C, and the results are shown in figure 6. In the condition B, it can be confirmed that the spray tip distance increases as the gas temperature rises. Since the spray impinges on the plate at an acute angle, the influence by the boiling region appears to be remarkable. In the condition A and D, spray tip penetration is constant regardless of gas temperature. Compared with the condition B, the shearing force acting on the droplet from the ambient gas increases in these conditions that the spray impinges perpendicularly to the plate. The spray tip penetration acts decreases since the evaporation of droplet is promoted by the rise in the gas temperature. However, as the gas temperature rises, the frictional resistance between the droplet and the plate surface decreases and the spray tip penetration increases. As a result, it is considered that the spray tip penetration became constant regardless of the gas temperature change. In the condition C, the spray tip penetration decreases as the gas temperature rises. Since droplets scattering from the upper side of the plate are pushed back to the gas flow, the influence by the boiling region is small. In addition, the evaporation of the droplet is most promoted since the shearing force by gas flow is the largest condition. Therefore, as the gas temperature rises, it is considered that small droplets evaporate early and the spray tip penetration decreases.

Table 1. Experimental condition

| Test liquid          |                   | Urea solution (32.5 wt%) |
|----------------------|-------------------|--------------------------|
| Liquid temperature   | $T_l$ [°C]        | 20                       |
| Nozzle type          |                   | 3-hole nozzle            |
| Nozzle diameter      | [ $\mu\text{m}$ ] | 120                      |
| Injection pressure   | $P_{inj}$ [MPa]   | 0.5                      |
| Injection quantity   | $Q_{inj}$ [mg]    | 83.3                     |
| Injection duration   | $t_{inj}$ [ms]    | 95.4                     |
| Injection cycle      | $f$ [Hz]          | 1                        |
| Injection number     | $n$               | 60                       |
| Gas temperature      | $T_g$ [°C]        | 250, 300, 350            |
| Gas velocity         | $V_g$ [m/sec]     | 10                       |
| Distance to the wall | $H$ [mm]          | 100                      |
| Wall angle           | $\theta_w$ [°]    | 0, 45                    |
| Injection angle      | $\theta_s$ [°]    | 45, 90                   |
| Sampling point       | $L$ [mm]          | 500                      |
| Sampling temperature | $T_s$ [°C]        | 113                      |

### Photography of Liquid Film and Deposit

Figure 7 shows the results of liquid film and deposit at 60, 150 and 210 seconds from the first injection. Figure 8 shows the results of the plate temperature in this case. It can be confirmed that the