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Numerical Investigation of the Evaporation and Mixing of UWS in a Diesel Exhaust Pipe

Tae Hyun Ahn, Gyo Woo Lee, Man Young Kim

***Abstract*—**Because of high thermal efficiency and low CO_2 emission, diesel engines are being used widely in many industrial fields although it makes many PM and NOx which give both human health and environment a negative effect. NOx regulations for diesel engines, however, are being strengthened and it is impossible to meet the emission standard without NOx reduction devices such as SCR (Selective Catalytic Reduction), LNC (Lean NOx Catalyst), and LNT (Lean NOx Trap). Among the NOx reduction devices, urea-SCR system is known as the most stable and efficient method to solve the problem of NOx emission. But this device has some issues associated with the ammonia slip phenomenon which is occurred by shortage of evaporation and thermolysis time, and that makes it difficult to achieve uniform distribution of the injected urea in front of monolith. Therefore, this study has focused on the mixing enhancement between urea and exhaust gases to enhance the efficiency of the SCR catalyst equipped in catalytic muffler by changing inlet gas temperature and spray conditions to improve the spray uniformity of the urea water solution. Finally, it can be found that various parameters such as inlet gas temperature and injector and injection angles significantly affect the evaporation and mixing of the urea water solution with exhaust gases, and therefore, optimization of these parameters are required.

***Keywords*—**Evaporation, Injection, Selective Catalytic Reduction (SCR), Thermolysis, UWS (Urea-Water-Solution).

I. Introduction

DIESEL engine is being used widely in many industrial fields, as it has high durability and thermal efficiency and low CO_2 emission. Compression ignition method of diesel engines, however, makes many particulate matter (PM) and nitrogen oxides (NOx) which give both human health and environment a negative effect in exhaust emission [1], and simultaneous reduction of these emissions is difficult due to trade-off of two compounds. Then, strengthened regulations such as EURO V and VI cannot be satisfied with pre-treatment technology. Therefore, the after treatment technologies are considered as a good solution to overcome the limit of pre-treatment technology.

PM is reduced by 90% by diesel particulate filter (DPF) which has already applied to vehicles [2]. On the other hand, SCR system is known as the best method to reduce NOx. Among many types of NOx reduction technologies such as LNT, LNC, and Urea-SCR, Urea-SCR is usually the famous one since the others have the problems such as poisoning by sulfur and treating dangerous gases [3]. As the evaporation and the thermal decomposition of urea water solution and spatial distribution of the reducing agent upstream the catalyst are crucial factors for the conversion of NOx, the dosing system has to ensure the proper preparation of the reducing agent at all operating conditions [4]. For this reason, on the basis of experimental result of Kim et al. [5], Birkhold et al. [6] conducted the numerical investigation to predict conversion and local distribution of the reducing agent in terms of the evaporation of water from a single droplet of urea water solution by using a rapid mixing and a diffusion limit models, which also examine the droplet motion and variable properties of the solution. Jeong et al. [7] carried out a study on effect of flow and NH_3 non-uniformities on the DeNOx performance and NH_3 slip in a Urea-SCR exhaust system, and compared multi-hole injector with one hole injector for NH_3 uniformity at the face of SCR monolith, while Choi et al. [8] performed the parametric study by changing swirl angle of the twin-fluid swirl type nozzle with angles of 0, 45, and 90 to find NOx reduction ratio with the swirl angles of the nozzle. Hwang et al. [9] conducted experimental study to analyze SMD (sauter mean diameter) and evaporation characteristic of the urea droplet, and ammonia uniformity index and NOx conversion efficiency with static mixer was measured. To our knowledge, however, study on the evaporation and thermal decomposition of the urea water solution needs to be continuously investigated, as each Urea-SCR system have different location, Injection condition, and the shape of the exhaust pipe.

In this work, therefore, temperature difference between inlet and outlet of exhaust pipe, NH_3 concentration, and spatial distribution of ammonia with a variety of inlet gas temperatures and spray conditions such as injector angle and spray cone angle were evaluated with the numerical approach. In the following, after kinetic parameters for the thermal decomposition model are determined comparing present simulation result with experimental and numerical results from Kim et al. [5] and Birkhold et al. [6], respectively, each spray condition will be compared through the comparison of estimated numerical value. Finally, some concluding remarks are presented.

II. Mathematical Models

A. Evaporation and Decomposition of UWS Droplets

Urea water solution (UWS, contains 32.5wt% urea; brand name: AdBlue) is sprayed into the hot exhaust stream to obtain the ammonia for which NOx can be converted into nitrogen and

Tae Hyun An is a graduate student in the Department of Aerospace Engineering, Chonbuk National University, Jeonju, Chonbuk 561-756, Republic of Korea.

Gyo Woo Lee is an Associate Professor in the School of Mechanical Design Engineering, Chonbuk National University, Jeonju, Chonbuk 561-756, Republic of Korea.

Man Young Kim is a Professor in the Department of Aerospace Engineering, Chonbuk National University, Jeonju, Chonbuk 561-756, Republic of Korea, (corresponding author; phone: +82-63-270-2473; fax:+82-63-270-2472; e-mail: manykim@jbnu.ac.kr).

water [10]. The subsequent generation of NH_3 in the hot exhaust gas proceeds in three steps [11], [12].

(1) Evaporation of water from UWS droplets

$$(NH_2)_2CO(aq) \rightarrow (NH_2)_2CO(s \text{ or } \ell) + 6.9H_2O(g) \quad (1)$$

(2) Thermolysis of urea into ammonia and iso-cyanic acid gases

$$(NH_2)_2CO(s \text{ or } \ell) \rightarrow NH_3(g) + HNCO(g) \quad (2)$$

(3) Hydrolysis of iso-cyanic acid into ammonia and CO_2 gases

$$HNCO(g) + H_2O(g) \rightarrow NH_3(g) + CO_2(g) \quad (3)$$

The decomposition mechanism of urea water solution to ammonia gas is illustrated in Fig. 1. In this figure, injected urea water solution droplets are heated up, and water in droplet surface evaporates first [12], subsequently, detached urea is turned into ammonia and iso-cyanic acid gases with thermolysis phenomena of urea, and finally, hydrolysis reaction changes generated iso-cyanic acid gas into ammonia gas by reacting water vapor. Since the evaporation and mixing of urea water solution and spatial distribution of the reducing agent upstream the catalyst are crucial factors for the conversion of NOx, the dosing system has to ensure the proper preparation of the reducing agent at all operating conditions.

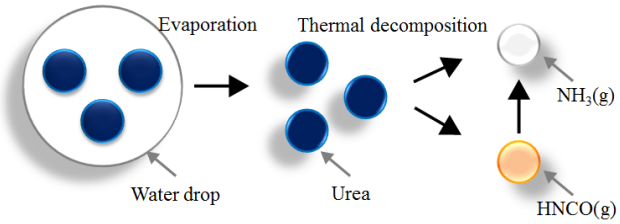


Fig. 1 Decomposition mechanism of urea water solution to ammonia

B. Numerical Procedure

For the numerical analysis of the injection of urea water solution, the models for evaporation and thermal decomposition are implemented into the commercial CFD code Fire 2011 which is based on the finite volume method by AVL [13]. In this commercial code, the fluid is treated with Eulerian flow, and the urea water solution droplets are examined with Lagrangian particle tracking approach [14], which solves the equation of motion for parcels of droplets with identical properties using the SCR-thermolysis model (SCR evaporation model including urea thermolysis) [13], and in this model, the thermolysis rate is defined by Arrhenius-type equation using kinetic parameters presented by Birkhold et al. [6]. Turbulence dispersion is defined by the Gosman-Ioannides model [15]. Between droplets and gas phase two-way coupling is considered for momentum, mass and heat transfer. For turbulence kinetic energy and dissipation one-way coupling is applied. And wall function was adopted to near the wall, because turbulent properties of the wall were rapidly changed.

Hydrolysis of HNCO in (3) is considered as a homogeneous gas phase reaction using the coupling interface of Fire to the CHEMKIN chemistry solver [16]. The used spray/ wall-interaction model of Kuhnke [17] which are influenced by the thermo-physical properties of the droplets accounts for dry and wet as well as for cold and hot walls by using dimensionless number. The film on the wall is modeled as a two-component fluid of urea and water coupled by momentum, species, and energy balances to the gas phase and the walls [18]. Internal flow is assumed for the three-dimensional turbulent flow of the compressible, reacting, and unsteady state to retain optimum evaporation and mixing characteristics of urea injected in Urea-SCR system. To address the physical significance of the present numerical solution data obtained from each cross section are compared with results measured from area-weighted average method [13].

Also, the spatial distribution of the NH_3 before the monolith entrance which affects the NO_x conversion efficiency [19], is evaluated by introducing uniformity index of ammonia concentration, γ, suggested by Weltens et al. [20], to confirm the uniform concentration distribution of reducing agent at the front face of the monolith as follows:

$$\gamma = 1 - \frac{1}{2n}\sum_{i=1}^{n}\frac{|C_i - \bar{C}|}{\bar{C}} \quad (4)$$

where, n, $\bar{C}$, and C_i are number of cells, mean concentration at the cross section, and local concentration at cell i, respectively. This uniformity index has value between 0 and 1, the higher uniformity index; the more uniform concentration distribution is obtained.

C. Computational Grid

Fig. 2 shows the side and isometric views of the computational grid system in the exhaust pipe with urea injector adopted in this work. Here, the angle between the entering and exiting exhaust pipe is 24.9°C, internal diameter is 55.5mm, and the length of the reactive region which is the distance between the injection point and the pipe outlet is 380mm. The injector is installed at the pipe wall, as directed into the flow with 3 different angles of -3, 15, and 45, respectively. All the numerical solutions are obtained by using the commercial software AVL Fire [13]. The grid system used in this work is composed of approximately 423,600 cells, and all numerical analysis are performed by using the same grid system.

D. Boundary and Injection Conditions

It is assumed that the flow of exhaust gas entering the system is fully developed, and the velocity and temperature fields obtained from the steady-state calculation were used as the initial condition of unsteady state simulation to predict the spray behavior of the urea water solution.

Exhaust gas passes through the exhaust pipe with mass flow rate of 40 g/s and inlet gas temperatures in set to 473, 523, and 573K, respectively. Exit pressure and heat flux are defined as 1 atm and 0 W/m^2, respectively. The injector has 3 holes, through

which urea water solution is injected with 33 different spray cone angles of 24, 37, and 50 and average SMD of 80μm. The urea water solution of 0.4g in 293K is injected into the hot exhaust stream with injection pressure of 5bar during 300ms from 0.4 to 0.7s.

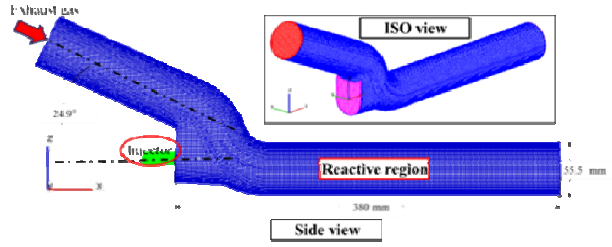


Fig. 2 Side and isometric views for the computational grid system of the exhaust pipe adopted in this work

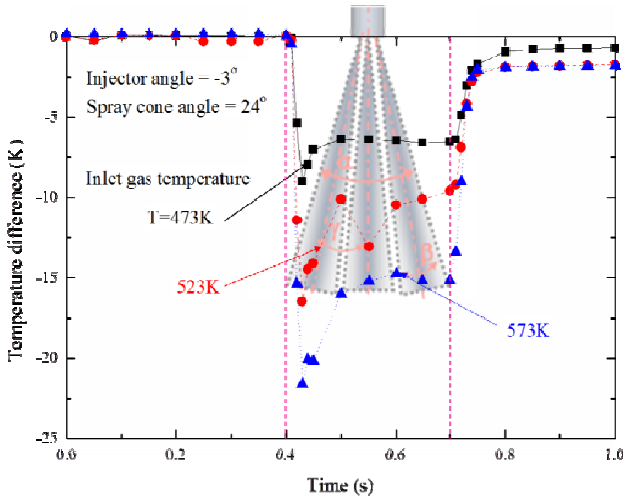
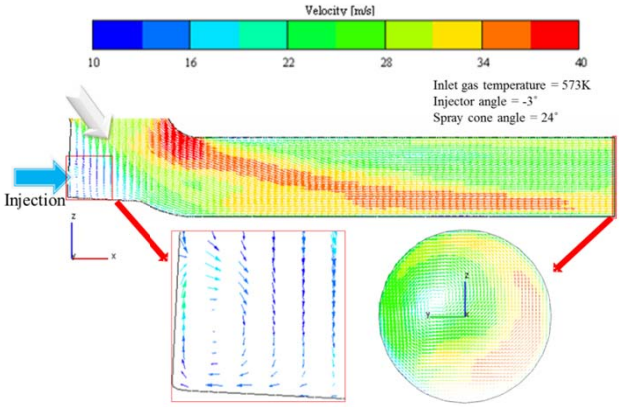


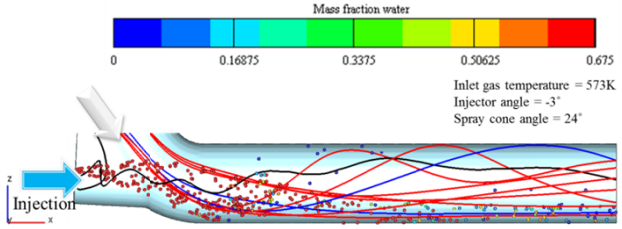
Fig. 3 Effect of inlet gas temperature on the temperature difference. The spray conditions are injector angle of -3 and spray cone angle of 24

III. Results and Discussion

In general, inlet gas temperature may significantly affect reaction rate of ammonia with NOx. To analyze the reaction characteristics of ammonia, firstly, effect of inlet gas temperature on temperature difference due to evaporation of UWSs between inlet and outlet exhaust pipes is investigated to find effect of inlet gas temperature. The spray conditions are injector angle of -3˚ and spray cone angle of 24˚. Urea water solution is injected into the exhaust pipe during 0.3s from 0.4 to 0.7s. As shown in Fig. 3, when the urea water solution is sprayed into the exhaust pipe at 0.4s, the temperature drop is occurred because thermal decomposition reaction consuming thermal energy (i.e. endothermic reaction) of urea solutions is occurred in hot exhaust environments [21]. The largest temperature difference at 0.42s is observed in all the cases of inlet temperature considered in this work. Also, it can be found that as the inlet gas temperature becomes high, the large temperature difference between inlet and outlet of the exhaust pipe occurs. When the spraying into exhaust pipe is over the exhaust gas temperature recovers its initial entering temperature.



(a) Velocity vector distributions



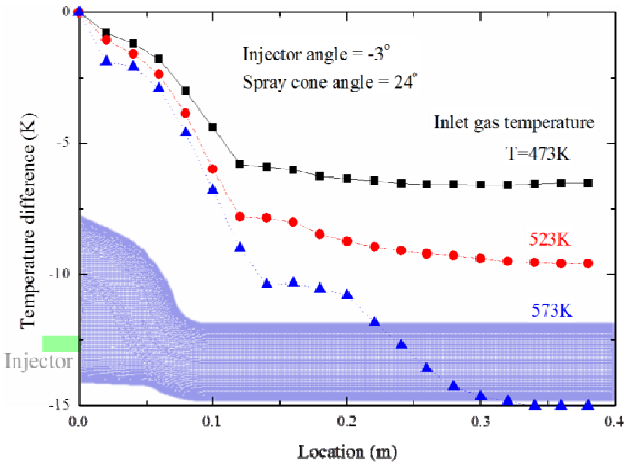
(b) Spray propagation and streaklines

Fig. 4 Numerical results at xz cross section of the exhaust pipe. The spray conditions are injector angle of -3 and spray cone angle of 24 at inlet gas temperature of 573K (t=0.7s): (a) Velocity vector distributions, (b) Spray propagation (droplets are colored with water fraction) and streaklines

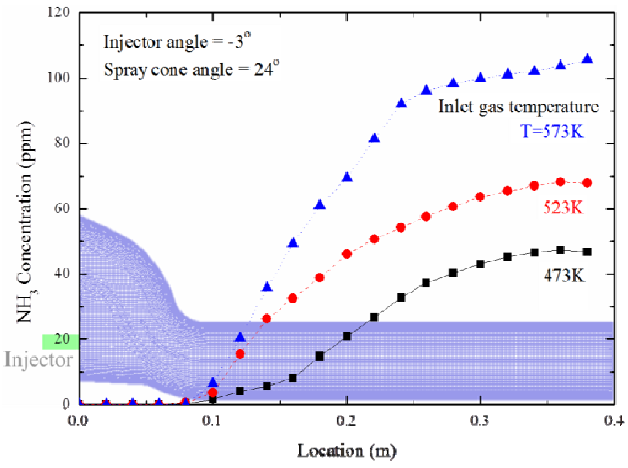
Fig. 4 represents the velocity vectors streaklines and spray behaviors at 0.7s. In this figure droplets are colored with water fraction at xz cross section. In the Fig. 4 (a), when the exhaust gas passes through a curved part of exhaust pipe, the swirl flow is observed and it can induce the mixing between UWS and exhaust gases. Also, it can be found that the main flow is directed to the lower pipe wall, and it makes most of the injected UWS moves along the lower pipe wall as shown in Fig. 4 (b).

Fig. 5 shows temperature and evaporated gaseous NH_3 distributions with the inlet gas temperature, injector angle, and spray cone angle of 573K, -3˚, and 24˚, respectively at xz and yz cross sections of the exhaust pipe at 0.7s. In the Fig. 5 (a), when urea water solution is injected into the exhaust gas at 573K, exhaust gas temperature is observed rapidly decrease about 550K. As can be seen in Fig. 5 (a), the temperature of the exhaust gas drops because the exhaust heat is consumed for evaporation of injected UWS. Especially, the temperature of exhaust gas near the injector is suddenly dropped to 550K. The tangential temperature distribution show that more temperature drop occurs because the injected UWS is mixed and evaporated

with exhaust gas as flowing downstream. Also, it can be found that tangential swirl flow makes cold point of the exhaust gas (i.e., evaporated NH_3 gas) flow along the pipe wall. Here, it can be confirmed that the evaporated NH_3 distribution is high at the pipe walls where gas temperature is relatively low since exhaust heat is consumed to evaporate the UWS.



(a) Exhaust gas temperature distributions



(b) NH_3 concentration distributions

Fig. 5 Effect of inlet gas temperature with location. The spray conditions are injector angle of -3 and spray cone angle of 24 (t=0.7s): (a) Temperature difference distributions, (b) NH_3 concentration distributions

IV. Conclusion

In this work, a three-dimensional numerical simulation of urea water solution injection has been conducted to evaluate the effects of inlet gas temperature and spray conditions on the temperature difference between inlet and outlet of exhaust pipe, ammonia concentration, and uniformity index of ammonia concentration distribution. An Eulerian-Lagrangian spray atomization model has been implemented into commercial code AVL Fire. The model validation was carried out by comparing present data with experiment and numerical data in literature. Also, the values estimated at the end of exhaust pipe are calculated by using area-weighted average method. The following conclusions can be drawn from this work.

(1) An increase in the inlet gas temperature increases temperature difference between inlet and outlet of exhaust pipe since evaporation and thermal decomposition reaction consuming thermal energy of urea particles are enhanced. Furthermore, an increase of temperature difference makes ammonia better generated due to endothermic reaction of urea particles.

(2) At the spray conditions of inlet gas temperature of 573K and spray cone angle of 24, the injector angle is found to have significant effects on both temperature difference and NH_3 concentration, and the maximum NH_3 quantity generated has been estimated more than twice than other installation angles.

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