Numerical Investigation on the Urea Deposit Formation Process in a Selective Catalytic Reduction System of a Diesel Engine Based on a Fluid–Solid Coupling Method

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ABSTRACT: Currently, selective catalytic reduction (SCR) systems have become an essential part in diesel engines, and urea crystallization is one of the most serious issues in SCR systems. In this paper, the urea deposit formation processes in the SCR system were investigated by numerical simulations based on a fluid–solid coupling method. The results show that the masses of the wall film and solid urea are larger at conditions with lower temperatures and higher injection rates. At higher temperatures, cyanate ions and ammonium ions are the most predominant compositions in the wall film, while at lower temperatures, solid urea is the main composition. It could also be deduced that the location of urea crystallization is more affected by the design of mixer at higher temperatures, whereas at lower temperatures, the location and installation angle of urea-water solution injector play a more important role.

1. INTRODUCTION

Due to the detrimental effects of diesel pollutants, regulatory agencies around the world are calling for increasingly stringent emission standards for diesel engines. In this respect, reducing diesel engine emissions is noteworthy.1 One group of the main emissions, which has been regulated in the emission standards is nitrogen oxides (NOx), which have negative effects on human body and natural environment.2 Currently, selective catalytic reduction (SCR) is the most promising postprocessing technology, which has been widely applied for the removal of NOx.3 In the SCR system, the urea–water solution (UWS) is injected into the exhaust gas upstream of the catalyst.4 After a series of physical and chemical processes (atomization and evaporation of the UWS spray, decomposition of urea, and hydrolysis of isocyanic acid), the sprayed UWS finally turns into ammonia (NH3), isocyanic acid (HNCO), and carbon dioxide (CO2) gases along with other solid compounds.5 NH3 is used as a reducing agent to convert NOx into harmless substances (N2 and H2O).6 However, the interactions between the UWS and the inner wall could cause damages to the SCR systems.7 Ideally, the urea in the SCR system is decomposed into only NH3 and CO2. Nevertheless, the impingement of UWS droplets on the wall of the SCR system is unavoidable. In this case, the wall is cooled by the UWS droplets and the wall film is formed. During the evaporation of the wall film, the wall temperature will be even lower due to the endothermic process; meanwhile, unexpected urea deposits composed of biuret, cyanuric acid (CYA), and ammelide may be produced on the mixer, inner wall, and substrate of the SCR system.8,9 When accumulation of urea deposition occurs, obvious increases in engine back pressure and decreases in conversion efficiency are accompanied, affecting the normal operation of the aftertreatment system and increasing fuel consumption.10–12 Thereby, mitigation of the urea
crystallization phenomenon has been regarded as the research focus of the SCR aftertreatment system.

Computational fluid dynamics (CFD) is an indispensable tool for the design and evaluation of urea deposit formation in the SCR system. Several numerical studies have been carried out to simulate the operation process and urea deposit formation of the SCR system. Zhang et al., Smith et al., Yi, and Zheng managed to simulate the in-cylinder flow field, wall film formation, and mixing characteristics in an SCR system. But the models they adopted were not validated for temperature distribution and the detailed decomposition processes of urea were not considered. Prabhu et al. applied a simplified urea thermolysis model to predict the behavior of urea deposit formation, whereas the detailed compositions of the urea deposit were neglected. Brack et al. incorporated a 15-step urea decomposition mechanism, Habchi et al. and Huang et al. integrated a 12-step urea decomposition mechanism into the CFD model and predicted the urea deposit formation process at different conditions. Since the key byproducts were considered in the decomposition mechanism, the compositions of the urea deposits could be analyzed in their studies. However, the changing rules of these byproducts were not systematically elaborated. As previously investigated, urea deposit formation were systematically investigated at different injection mass rates of UWS. The variations in the compositions of urea deposits were also studied in depth.

In this paper, a CFD model, which has wall film model, spray breakup model, detailed urea decomposition model, and fluid—solid coupling model integrated in it, was built to study the operation of an SCR system. The model was validated against pressure drop data and temperature measurements of both inner gas and the outer wall. Based on the model, the in-cylinder flow field, temperature distribution, film formation, and urea deposit formation were systematically investigated at different operating points and different injection mass flow mass rates of UWS. The variations in the compositions of urea deposits were also studied in depth.

2. EXPERIMENT SETUP AND NUMERICAL METHODS

2.1. Numerical Methods. In this paper, the construction of the CFD model for the SCR system of a diesel engine was based on Converge software. The breakup of the UWS droplets was calculated by the Taylor analogy model, which treats the UWS droplet as a spring-mass system based on eqs 1–6. The information of UWS droplet size distribution shown in Figure 1 was obtained from experiments.

The evaporation of water from UWS is predicted based on the nonrandom two-liquid equation. After all of the liquid water is evaporated from UWS, solid urea is left and the decomposition of urea is initiated. To take the formation of the byproducts into consideration, the detailed decomposition kinetic mechanism adopted in the study of Habchi et al. was adopted for the thermolysis of urea as well as the formation of biuret, CYA, and ammelide.

$$F - kx - dx = mx$$

Figure 1. Measured diameter size distribution of UWS droplets.

Table 1. Engine Specifications

| item                  | specifications |
|-----------------------|---------------|
| number of cylinder    | 4             |
| engine type           | turbocharged, water cooled |
| bore × stroke (mm²)   | 105 × 130     |
| displacement (L)      | 4.5           |
| rated power (kW)      | 110           |
| rated speed (rpm)     | 2300          |
| idle speed (rpm)      | 650           |

Figure 2. Layout of the engine test bed.

Table 2. Engine Operation Conditions for Model Validation

| experimental operating conditions | engine speed (rpm) | exhaust gas mass flow (kg/h) | engine torque (N·m) | inlet temperature (K) | outlet temperature (K) |
|-----------------------------------|--------------------|-------------------------------|---------------------|-----------------------|------------------------|
| OP#1                              | 1600               | 265                           | 216                 | 639                   | 614                    |
| OP#2                              | 1600               | 258                           | 177                 | 598                   | 575                    |
| OP#3                              | 1600               | 245                           | 134                 | 553                   | 535                    |
| OP#4                              | 1600               | 240                           | 98                  | 511                   | 497                    |
| OP#5                              | 1600               | 236                           | 63                  | 470                   | 460                    |
where \( x \) is the displacement of the droplet from its equilibrium position, \( \rho_\text{l} \) and \( \rho_\text{g} \) are the densities of liquid and gas, \( u_i \) is the relative velocity between the droplet and the gas, \( r_0 \) is the droplet radius, \( \sigma \) is the gas–liquid surface tension coefficient, \( \mu_\text{l} \) is the droplet viscosity, and \( C_F, C_K, \) and \( C_d \) are empirical constants. It is assumed that the droplet is broken only if \( x > C_b r \), where \( C_b \) is an additional infinite number. \( x \) could be made dimensionless by \( C_b r \).

Breakup occurs only if \( y > 1 \). For low-damping droplets, if the relative velocity is assumed to be constant, the value of \( y \) can be determined by eq 5. \( y \) could be further described by the following formula:

\[
y(t) = W_\xi + \epsilon^{1/4} \left[ (y - W_\xi) \cos(\omega t) \right] + \frac{1}{\omega} \left( \frac{dy}{dt} (0) + \frac{y(0) - W_\xi}{t_d} \right) \sin(\omega t)
\] (6)
where

$$W_{\varepsilon} = \frac{\rho \mu^2 \tau_0}{\sigma} \quad (7)$$

$$W_{\kappa} = \frac{C_F}{C_k} W_{\varepsilon} \quad (8)$$

$$\frac{1}{t_d} = \frac{C_d}{2} \frac{\mu_1}{\rho_1 \tau_0} \quad (9)$$

$$\omega^2 = \frac{C_k}{\rho \tau_0} - \frac{1}{t_d} \quad (10)$$

In eq 6, $\omega$ is the vibration frequency of the UWS droplet. In eq 7, $W_{\varepsilon}$ is the Weber number, $C_F$, $C_k$, and $C_d$ are constants determined by the comparison between experimental and theoretical results.

In SCR systems, the gas-phase reactions for the oxidation of NH$_3$ as well as the formation and destruction reactions of NO$_x$ are less significant. Thereby, the detailed nitrogen chemistry proposed by Glarborg et al.\textsuperscript{24} with 46 species and 283 reactions has been reduced to a shorter version with 22 species and 113 reactions by the directed relation graph method with error propagation (DRGEP) reduction method.\textsuperscript{25} Afterwards, the version with 22 species was further reduced to the final version with 19 species and 64 reactions by full species sensitivity analysis (FSSA) reduction method\textsuperscript{26} to describe the variations in the mole fractions of the gaseous species in the SCR system.

To achieve efficient and accurate fluid–solid coupling, the supercycling method was utilized for the heat transfer between the fluid and solid phase. The supercycling method was carried out according to the following steps:

(a) Solve the fluid and the solid together with the transient solver; then, store the heat transfer coefficients and the wall temperatures at the fluid–solid interface.

(b) Freeze the fluid solver and calculate the time-averaged heat transfer coefficients, which are treated as the boundary conditions at the fluid–solid interface.

(c) Solve the solid temperatures until the steady state is reached.

(d) Update the solid temperature field and unfreeze the fluid solver.

(e) Repeat step (a) to step (d) until the solid temperature converges.

### 2.2. Setup of the Engine Test Bed and Model Validation

An engine test bed with an aftertreatment system was built to verify the numerical model. The main specifications of the test engine are given in Table 1. The setup of the test bed is shown in Figure 2. For the evaluation of the urea deposit characteristics, the SCR postprocessing system was designed to be detachable. Thermocouples and pressure transducers were installed at different locations of the SCR system to collect the corresponding temperatures and pressures (CYB4211-500G...
with accuracy of ±0.1 kPa). There are two kinds of thermocouples, one for the measurement of gas temperatures (K type with accuracy of ±0.25%) and another for the measurement of wall temperatures (Omega WTK-8-60 with accuracy of ±0.25%).

The numerical model was verified under five different operating conditions. The specific parameters of the five operating conditions are shown in Table 2. During the experiments, five monitor points of temperatures were set up. The locations of these monitor points are provided in Figure 3. Two of the monitor points were set for the measurement of local gas temperatures (monitor point 2 and monitor point 5), and the rest of the monitor points were set for the measurement of wall temperatures (monitor point 1, monitor point 3, and monitor point 4). The first, third, and fourth monitor points were located on the outer wall before the mixer, the outer wall around the first SCR substrate, and the outer wall around the muffler, respectively. The second monitor point is located in front of the first SCR substrate and the fifth monitor point is located in the exhaust pipe after the outlet of the SCR system.

Figure 4 shows a comparison between the experiment and simulation values of the wall temperatures, gas temperatures, and pressure drops at different engine operating conditions. The data indicated the simulation results fit well with the experiment results. Though there are some errors between the experiment and simulation results, all of the errors are within ±5.0%. This proves that the present model is reliable and confirms that it could be used for further simulation.
3. RESULTS AND DISCUSSION

3.1. Wall Film and Urea Deposit at Different Conditions. To investigate the mixing quality, film, and urea deposit formation characteristics in the SCR system, transient simulations were conducted at different injection rates of 300, 400, and 500 mg/s. As injection frequency has profound effects on the wall film and urea deposit formation, the injection frequency was fixed at 1 Hz and the corresponding simulation time was fixed at 1 s for all of the simulation cases to eliminate its effects. Figure 5a provides the accumulated and transient film masses at the end of the injection cycle with various injection rates. The accumulated film mass refers to the total liquid film mass that has interacted with the inner walls since the beginning of the simulation. The transient mass refers to the transient total liquid film mass on the inner walls. It could be observed from the figure that the accumulated and transient film masses are higher at conditions with lower exhaust temperatures and higher injection rates. This is because the formation of the wall film is closely related to the evaporation of UWS droplets. The evaporation of UWS droplets is slower at low-temperature conditions, and an increased amount of UWS is introduced into the exhaust system at higher injection rates, leading to increased film mass. At operating points with relatively higher temperatures, the variations of solid urea, biuret, CYA, and ammelide with the increases of injection rate are similar to those of the wall film, i.e., the masses of these species would increase with the increase of the injection rate (Figure 5b,c). At operating points with relatively lower temperatures, the trends of solid urea with the variation of injection rate are still consistent with those of the wall film, whereas the trends of biuret, CYA, and ammelide are different from those of the wall film. As could be observed, the masses of biuret, CYA, and ammelide vary slightly with the change of the injection rate at operating conditions with lower exhaust temperatures. This could be explained by the longer time needed for the evaporation of water in UWS at higher injection rates, leaving less time for the formation of biuret, CYA, and ammelide. In this case, though an increased amount of UWS is injected, the masses of biuret, CYA, and ammelide, which require a longer time for generation, will not substantially increase. Besides, as demonstrated in Figure 5b,c, the highest masses of biuret, CYA, and ammelide appear at OP#1 and OP#3, indicating that conditions with too high or too low temperatures are not favorable for the production of urea decomposition byproducts.

Figure 5d gives the percentages of different compositions in the wall film at the end of the injection cycle. At higher temperatures (OP#1 and OP#2), cyanate ion (NCO\(^{-}\)), ammonium ion (NH\(_4\)\(^{+}\)), solid urea, and CYA are the most predominant compositions in the wall film, while at lower temperatures (OP#3 to OP#5), solid urea, water, cyanate ion (NCO\(^{-}\)), aqueous urea, and ammonium ion (NH\(_4\)\(^{+}\)) have higher fractions. As illustrated, the fraction of solid urea declines with the increase of exhaust gas temperature. This is because at high

Figure 8. Simulated wall film distribution of different operating points at the end of the injection cycle with an injection rate of 400 mg/s: (a) OP#1, (b) OP#2, (c) OP#3, and (d) OP#5.
temperatures, solid urea is easier to decompose to NCO$^-$ and NH$_4^+$, leading to a reduced fraction of solid urea along with increased fractions of NCO$^-$ and ammonium ion (NH$_4^+$). Moreover, higher fractions of aqueous urea and water exist in the wall film at low-temperature conditions as a result of the increased time for the complete evaporation of UWS droplets. It could also be noticed from Figure 5d that the percentages of the hydrogen ion (H$^+$) and biuret are lower than 5% at most conditions. Biuret is produced from solid urea; it could be continuously converted into CYA and ammelide, thus little biuret could be left in the urea deposit if the retention time in the aftertreatment system is not long enough. In light of H$^+$, it could easily react with NCO$^-$ and water, turning into gas species including NH$_3$ and CO$_2$. Thereby, the fraction of H$^+$ is extremely low at all conditions.

Figure 6 presents the accumulated and transient film masses at different operating points with an injection rate of 400 mg/s. It can be found from the data that both the accumulated and transient film masses are higher at conditions with lower exhaust temperatures during the whole injection cycle. At OP#2 to OP#5 with the exhaust temperature ranging from 197 to 325 °C (470 to 598K), the accumulated and transient film masses increase rapidly during the period from 0.03 to 0.1 s of the injection cycle, indicating that the formation of the wall film occurs during the injection process of UWS and shortly after the UWS injection process. This is because after UWS is injected into the exhaust system, it will first experience atomization and evaporation. In this case, part of the UWS droplets are transformed from liquid phase to gas phase. The UWS droplets, which are left after the evaporation process, could travel through the exhaust gases and contact with the wall of the SCR system, leading to the formation of the wall film on the wall surfaces. At OP#1, as the temperatures of gas and wall are relatively high, the evaporation of the UWS droplets will be strongly accelerated; the increase of accumulation and transient film mass will rise slowly during the period from 0.1 to 0.4 s of the injection cycle after the start of the injection.

Figure 7 provides different compositions of urea deposits during the injection cycle. As illustrated, the mass of solid urea increases rapidly during the period from 0.03 to 0.2 s of the injection cycle at OP#1 to OP#5. It can be found that the periods with a high increasing rate of solid urea are longer than those of the wall film. This is because solid urea is formed after water is evaporated from UWS droplets, which means more time will be consumed for the formation process of solid urea. At higher temperatures, the evaporation of water is accelerated and the decomposition of solid urea is faster than the formation of solid urea in the later stages of the injection cycle. Thereby, the mass of solid urea experiences a first increase and then decrease trend during the whole injection cycle. At lower temperatures, the evaporation of water will be much slower and the decomposition of solid urea will be restrained, leading to a
continuously increasing trend during the injection cycle. In view of biuret, an increasing trend with time could be observed at most operating points. However, at OP#2, fluctuations of biuret mass are demonstrated. This behavior could be explained by the fierce competition between the formation and decomposition reactions of biuret at this condition. Since the formation of CYA and ammelide is later than the formation of solid urea and biuret, the masses of these two species exhibit a monotonically rising trend during the whole injection cycle.

Figure 8 shows the wall film distribution of different operation points at the end of the injection cycle. It can be seen that the locations for the wall film are the same for operating points with higher exhaust gas temperatures. There are two major locations for the accumulation of the wall film at these operating points (OP#1 to OP#3), i.e., around the injector and before the first substrate. Nevertheless, at OP#5, the wall film accumulates on the inner surface of the mixer and the wall surface below the mixer. Since solid urea and solid byproducts formed during urea decomposition are formed from UWS, the distribution of these species is similar to that of the wall film (Figure 9). It should also be noticed by comparing Figures 8 and 9 that the accumulation of wall film and solid urea is easier at conditions with lower temperatures.

Figure 10. Simulated velocity distribution of different operating points with an injection rate of 400 mg/s: (a) OP#1, (b) OP#2, (c) OP#3, and (d) OP#5.
3.2. Velocity and Temperature Distribution at Different Conditions. Figure 10 demonstrates the velocity distribution of different operating points during the UWS injection process. At all operating points, regions with highest velocities are distributed at the inlet pipe and the outlet pipe due to the smaller diameters. After the exhaust gas flows into the SCR system, the gas flow is blocked by the mixer, which means a part of the inlet gas will flow backward to the regions around the injector. Thus, part of the injected UWS droplets could be influenced by the motion of the flow and travel to the regions around the injector. This explains why the formation of the wall film and urea crystallization could be found at these regions. At operating points with higher temperatures, the masses of the UWS droplets are smaller and the mass flow rates of the exhaust gas are higher. In this case, the UWS droplets are easier to be carried away by the exhaust gas flow and accumulate near the

Figure 11. Simulated temperature distribution of the SCR system at different operating points with an injection rate of 400 mg/s: (a) OP#1, (b) OP#2, (c) OP#3, and (d) OP#5.
injector. At operating conditions with lower temperatures, the masses of the UWS droplets are higher and the mass flow rates of the exhaust gas are lower; the movement of the UWS droplets is more dominant by the installation location and angle of UWS injector. Therefore, the wall film and urea crystals appear at surfaces opposite to the injector.

Figure 11 provides the temperature distribution at different operating points. As shown, the regions with lower temperatures are mainly distributed at regions near the inner walls of the SCR system, near the circular part of the mixer, and near the injector. It could also be noticed that the temperatures of the near-wall regions before the substrates are lower at the bottom side due to the cooling effects of the UWS droplets. At operating conditions with higher temperatures, the inner wall temperatures of the SCR system are generally higher than 450 K, which is easier for the decomposition of the urea crystals. At operating conditions with lower temperatures, the inner wall temperatures of the SCR system are lower than 450 K, which restrains the evaporation of the wall film and the decomposition of urea crystals. Thereby, it could be deduced that during the operation of a realistic engine, urea crystallization tends to appear at the inner wall near the injector, the inner wall below the mixer, and the bottom part inside the mixer. This conclusion could be further confirmed by the temperature distribution of the mixer, as shown in Figure 12.

Since the bottom part inside the mixer has more possibilities to make contact with UWS droplets, the temperatures at these regions are obviously lower, which, in turn, increases the tendency for urea crystallization. It could also be found from Figure 12 that at operating conditions with lower temperatures and lower mass flow rates of exhaust gas, the low-temperature regions of the mixer are more concentrated and the areas of the low-temperature regions are larger, suggesting that there are more possibilities for the formation of the wall film and urea crystals at the bottom part inside the mixer at low-temperature conditions. These results are consistent with the results in Figures 8 and 9. Once the low-temperature operation time is sufficient, the amount of urea crystals could block up the holes of the mixer, leading to increased pressure drop and more serious urea crystallization.

3.3. NH₃ and HCNO Distribution at Different Conditions. Figure 13 shows the distribution of NH₃ and HCNO before the SCR substrate of different operating points at the end of the UWS injection process. It is obvious that the concentrations of NH₃ and HCNO are higher at operating
conditions with higher exhaust temperatures. NH\(_3\) mainly comes from the decomposition of NH\(_4^+\) and hydrolysis of HNCO. Both of these reactions could be promoted at high temperatures, leading to a substantially higher production rate. HNCO is predominantly produced from the decomposition of urea, which is also temperature dependent. Thereby, the formation of HNCO could also be promoted at higher temperatures. As HCNO could be converted to NH\(_3\) with the presence of water, the concentrations of NH\(_3\) are markedly higher than those of HCNO. Influenced by the flow field, the gas species will be concentrated in the upper part of the substrate at OP\(_1\) to OP\(_3\). The distribution of gaseous species indicates that the surface reaction processes at the lower part of the substrate may be restrained by the lack of reductant at these conditions. This behavior, however, is not true at lower temperatures as the UWS droplets and NH\(_3\) are concentrated in the lower part of the substrate; additionally, the regions with high in this case, it could be deduced that the lower conversion efficiencies of the SCR system at low-temperature conditions could be attributed to both the lower reaction rate of the surface reactions and the worse mixing quality.

4. CONCLUSIONS
This paper aims to investigate the wall film and urea deposit formation processes by numerical simulations based on the fluid–solid coupling method. The key findings are as follows:

(1) Numerical simulations based on the fluid–solid coupling method could reproduce gas and wall temperatures with high accuracy, indicating that the urea deposit formation process could be predicted precisely.

(2) At the end of an injection cycle, accumulated and transient masses of the wall film along with the mass of solid urea are higher at conditions with lower exhaust temperatures and higher injection rates. The masses of urea decomposition byproducts with higher molecular weights show a first increasing then decreasing trend with increasing exhaust temperature. At conditions with sufficient high temperatures, the masses of urea decomposition byproducts with higher molecular weights increase with the increase of the injection rate, while at low-temperature conditions, the masses of urea decomposition byproducts vary slightly with the injection rate.

(3) The locations of the wall film and urea crystals are highly dependent on the design of mixer at conditions with higher temperatures, whereas they are more associated with the location and installation angle of the UWS injector at conditions with lower temperatures.

(4) The concentrations of gas species, including NH\(_3\) and HNCO, are higher at conditions with higher temperatures. The mixing quality is also better at conditions with higher temperatures, suggesting that in addition to low reaction activity, the slow evaporation and poor mixing at low-temperature conditions are also important reasons for the low conversion efficiencies of an SCR system at low-temperature conditions.

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Figure 13. Simulated distribution of NH\(_3\) and HNCO (before substrate) at different operating points with an injection rate of 400 mg/s: (a) OP\(_1\), (b) OP\(_2\), (c) OP\(_3\), and (d) OP\(_5\).
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Notes
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ABBREVIATIONS
CFD, computational fluid dynamic; CYA, cyanuric acid; DRGEP, directed relation graph method with error propagation; FSSA, full species sensitivity analysis; SCR, selective catalytic reduction; UWS, urea–water solution

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