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Numerical Modeling of Sublimation of Ammonium Carbamate Applied to Supply System of NOx Reductant

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Abstract: Recently, ammonium carbamate (AC) has attracted attention as a substitute for urea, which is a commonly used reductant for NO_x emitted from combustion engines. The AC exists as a solid at room temperature, and it is decomposed to NH₃ and CO₂ gases by heating. Therefore, adequate heat transfer is an essential issue in the design of AC pyrolysis reactor. In this study, a numerical model that describes the sublimation of AC was developed. For modeling, this study considered the three different calculation zones: solid-phase zone, gas-phase zone, and sublimation zone. Additionally, during the sublimation process, collapse of upper solid AC into the hollow space below by the effect of gravity is considered. As a result, it is presented that the modeling shows reasonable information about the AC sublimation in a reactor, such as temperatures in a reactor, pressure of reactor, and flow rate of sublimated gas. However, it is also found that accurate prediction of spatial temperature distribution is challenging because it is related to the accurate prediction of the internal shape of AC and its collapse in a reactor.

Keywords: ammonium carbamate; sublimation; numerical method; ammonia; NOx

1. Introduction

As one of the major sources of air pollutants, NO_x emissions have been strictly regulated. [1]. However, approximately 500 million tons of NO_x are still emitted annually from vehicles worldwide [2], affecting the quality of human life. Selective catalytic reduction (SCR) has been the most commonly used technology to reduce NO_x emissions from vehicles [3,4]. The SCR refers to a catalyst system that converts NO or NO₂ into N₂ and H₂O by reacting with NH_3 , and it shows an exceptionally high NO_x reduction efficiency and high system reliability. However, NH_3 is needed as a NO_x reducing agent in the SCR. It is a toxic substance and very dangerous in the event of a leak. Additionally, it is difficult to store in a liquid or gaseous state. Therefore, many vehicles currently use urea $(CO(NH_2)_2)$ water solution to supply NH₃. The urea water solution is decomposed into NH₃ and CO₂ when it is sprayed onto high-temperature exhaust gases. However, effective decomposition of urea solution usually requires a high exhaust gas temperature of 200 °C or more [5]. Due to this requirement, a substantial amount of NO_x is emitted during low temperature operating conditions [6]. One of the other disadvantages is that the urea solution can freeze below $-12 \,^{\circ}C$ [7]. Additionally, it is not easy to keep the uniform distribution of ammonia in a catalyst during transient engine operating conditions [8].

The AC (ammonium carbamate, $H_2NCOONH_4$) has been proposed as an alternative of urea [5]. The AC can be sublimated from solid to gas mixture of NH_3 and CO_2 at temperatures (approximately 60 °C at 1 atm) lower than those for urea. Another advantage of AC is that the storage capacity of NH_3 is about three times larger than that of urea



Citation: Woo, S.-H.; Noh, J.-H.; Raza, H.; Kim, H. Numerical Modeling of Sublimation of Ammonium Carbamate Applied to Supply System of NOx Reductant. *Energies* 2021, *14*, 3795. https:// doi.org/10.3390/en14133795

Academic Editor: Mejdi Jeguirim

Received: 17 May 2021 Accepted: 21 June 2021 Published: 24 June 2021

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Copyright: © 2021 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). solution. Besides, the NH₃ gas produced from AC has better mixing characteristics with exhaust gas than that of urea solution. In general, AC is stored in a reactor. The reactor's pressure increases when it is heated because some amount of AC is sublimated in the reactor. Then, the NH₃ gas is injected into the exhaust gas using the elevated pressure [5]. However, it is difficult to control the sublimation rate of AC because of spatially uneven distribution of AC mass and temperature in the reactor. For example, the AC contacting with the heat sources is sublimated at first, and a gas space is created there. After that, the AC that exists spatially apart from the heat sources is sublimated by the effect of convective heat transfer. Such a temporally and spatially complex sublimation process results in a non-uniform sublimation rate. Therefore, optimal design of the reactor is necessary to control the sublimation rate effectively. Previous researchers have investigated the simple design parameters of AC reactor only by experimental methods [9–11]. However, it was not easy to clearly understand the heat and mass transfer phenomena in the reactor. Such difficulties hinder the optimal design of the reactor.

Many numerical models have been developed to solve engineering problems of phase change from solid to liquid [12–14] or liquid to gas [15,16]. However, numerical models for phase change from solid to gas have not been proposed well, because it is not a common phenomenon encountered in engineering problems. Kim et al. [17] developed a numerical method to investigate the frosting of water. They tried to predict the variation of heat transfer coefficient owing to the frost. They also simulated the growth of frost by the deposition of H₂O molecules in the air on a cold surface. Zhang et al. [18] calculated the amount of heat energy removed by sublimation, evaporation, and freezing that occurred on a porous plate, which was soaked in the water. However, the porous plate's shape did not vary, and only the heat and mass transfer were analyzed. Zadravec et al. [19] investigated the variation of the interface height by simulating the material's freeze-drying process in a vial. However, this study considered only the height of the interface. It was not developed to interpret the three-dimensional sublimation phenomenon. As seen above, there have been many simulation studies on the phase change from gases to solid or solid to gases. However, as far as we know, there are no three-dimensional simulation studies about AC sublimation. This seems to be because AC is the newly introduced material for ammonia storage.

This study's objective is to develop a numerical model, which simulates the sublimation of AC for use in the optimal design of a reactor.

2. Materials and Methods

2.1. Experiment Set-Up

Experiments on AC sublimation were conducted to verify the numerical model developed in this study. As shown in Figure 1, the experimental apparatus is divided into three parts: AC reactor (pyrolysis space), heated water supply device, and heated air supply device. The water heated at 90 °C is circulated outside the reactor to supply heat. Two glass plates are installed on the top ceiling of the reactor to visualize the shape of solid-phase AC. The hot air heated to 120 °C is supplied between the two glass plates to prevent the re-solidification of NH₃ and CO₂ gases on the surface of the glass plate. In the AC reactor, four fins are installed to enhance heat transfer characteristics. Five thermocouple rods (TRF1, TRF2, TRF3, TRA1, TRA2) are installed in the reactor to measure temperature distribution. TRF1, TRF2, and TRF3 are installed near a fin that are expected to sublimate first. TRA1 and TRA2 are installed in the middle between two fins that are expected to sublimate later. In each of the rods, four thermocouples are implanted at regular intervals. The entire experimental apparatus is covered with insulation material.

The AC exists in the form of powder. However, when it is exposed at a certain condition for a long time, the AC may harden and agglomerate. In this study, the AC was crushed into small powders before the tests.

 NH_3 and CO_2 gas mixtures were exhausted from the bottom of the vessel. The pressure was measured using a pressure sensor (PSH, Sensys, Korea) at the outlet. In the

experiment, after 30 min of warm water circulation, the outlet valve was opened, and the flow rate of gas was measured by MFC (mass flow controller). The outlet gas line was heated to 120 °C to prevent clogging, owing to the re-solidification of NH₃ and CO₂ gases.



Figure 1. Schematic of experimental set-up for validation of AC sublimation model.

2.2. Numerical Method

2.2.1. Sublimation Numerical Analysis Model

Three kinds of calculation zones are considered in the numerical model developed in this study: solid-phase zone, gas-phase zone, and sublimation zone. Only solid AC is present in the solid-phase zone. The gas-phase zone also only contains gases. The sublimation zone is a region where the temperature reaches the critical temperature for sublimation. Both solid and gas exist in the sublimation zone.

The temperature of every zone is monitored at each iteration of the calculation to classify the zone. When the zone's temperature is higher than the sublimation critical temperature (T_{th}), the solid zone transforms into a sublimation zone. Here, the T_{th} is determined by the Figure 2, which is obtained from an experiment of reference [9]. The solid-phase and gas-phase mass ratio in the zones (ρ_s) is calculated at each iteration of calculation to classify the zone. When one mole of solid AC is pyrolyzed, one mole of CO₂ and two moles of NH₃ gas are generated. Generated CO₂ and NH₃ gas are considered by source term of fluid in the sublimation zone. If ρ_s is decreased to zero, the sublimation zone transforms to a gas-phase zone. In the gas-phase zone, conservation equations of computational fluid dynamics (CFD) are applied to calculate the conserved variables.

Figure 3 shows the concept of a model that explains how to simulate the change in shape of a solid AC where sublimation occurred. Figure 3 is expressed two-dimensionally for ease of understanding, but the real model was calculated three-dimensionally. Step 1 is the initial step at Time *i*. The distinction between the solid-phase and gas-phase zones is evident, and there is no sublimation zone. Step 2 is the heating stage. The solid-phase zone is transformed to the sublimation zone when the cell temperature (T_s) is greater than the sublimation critical temperature (T_{th}). The mass ratio of solid-phase and gas-phase (ρ_s) is also calculated in Step 2. In Step 3, the sublimation zone's cell transforming to the gas-phase zone is determined based on the ρ_s . In Step 4, the solid phase zone is shifted in the direction of gravity to fill the voids created by the phase transformation. It was assumed that solid AC was in powder form, as it had weak bonding forces, and it shifted in the direction of gravity without plastic action. Steps 1–4 are repeated until the residue converges below a specific value. Furthermore, the time step is shifted forward from *i* to *i* + 1. For the next time step, the zone information (solid, gas, sublimation) calculated in the

previous iteration is used as the initial value. In this study, the amount of sublimated AC, the pressure of the pyrolysis vessel, and the amount of NH_3 gas generated are predicted by continuing this calculation procedure.



Figure 2. Equilibrium pressure of AC with respect to the temperature measured in a closed chamber [9]. Reprinted with permission from ref. [9]. Copyright 2021 Elsevier.



Figure 3. Concept of the model: Changes in the shape and location of solid AC where sublimation occurs due to heat transfer.

A commercial CFD program ANSYS FLUENT 19.2, was used in this study. The general mass, momentum, and energy conservation equations of the commercial program were used. As a turbulent model, the standard k– ε model was used. The latent heat of sublimation of AC, S_e , was added to the energy equation as follows:

$$\frac{\partial(\rho c_p T)}{\partial t} + \nabla \cdot \left(\rho c_p T\right) = -\nabla(k \nabla T) + S_e, \tag{1}$$

where ρ is the density, c_p is the specific heat, *T* is the temperature, *k* is the thermal conductivity. The generation of NH₃ and CO₂ gases by AC sublimation is incorporated in the species transport equation as follows:

$$\frac{\partial(c_k)}{\partial t} + \nabla \cdot (c_k u) = -\nabla (D_k \nabla c_k) + S_k$$
(2)

where c_k is the concentration of each species, u is the velocity, D_k is the diffusion coefficient of each species, and S_k is the source term for each species generation. The NH₃ and CO₂ gases generated by AC sublimation are calculated in terms of S_k .

Properties of gases and solid material of reactor are listed in Table 1 which are mainly citing NIST (National Institute of Standard and Technology) data. The sublimation heat of solid AC is 159.94 kJ/mol [20].

Description		Density [kg/m ³]	Viscosity [Pa-s]	Specific Heat [J/kg-K]	Thermal Conductivity [W/m-K]
Fluid	Air	0.898	2.264×10^{-5}	1011	0.032
	Ammonia	0.689	$1.015 imes 10^{-5}$	2158	0.025
	Carbon Dioxide	0.730	$1.801 imes 10^{-5}$	908	0.022
	Water	965.3	$0.315 imes10^{-3}$	4206	0.675
Solid	SUS 304	7930	-	502	16.2
	Insulator (Urethane)	70	-	1045	0.026
	Ammonia Carbamate	1380	-	1670	2.0
	Glass	2800	-	750	0.7

Table 1. Physical properties of working fluid and solid.

Commercially available ANSYS Fluent 19.2 software (Canonsburg, Pennsylvania US) was used. Sublimation of solid AC was calculated by a user-defined function. The calculating elements numbered from 1.1 million to 1.7 million were tested for grid independence, and the number of elements was decided to about 1.3 million. The coupled governing equations were discretized using the finite volume method and solved with SIMPLE algorithm. For actual analysis, convergence conditions of solution were taken to be less than 10^{-5} of relative uncertainty level.

2.2.2. Model Validation

The sublimation model developed in this study was verified by comparing it with experimental results. As shown in Figure 4, the calculating area is identical to the pyrolysis space inside the AC reactor. The inlet boundary conditions of air supplied to the space between the two glass plates are as follows: the temperature is 120 °C, and the velocity of flow is 1 m/s, respectively. The inlet boundary conditions of warm water for supplying heat are a temperature of 90 °C and a flow rate of 5 L/min. All the outlet boundary conditions, such as the heating air, vessel's outlet, and the warm water outlet, are set as the pressure outlet. All the boundary conditions of the outside wall (except the top of the glass) are set as adiabatic conditions. The glass plates at the top of the experimental apparatus are exposed to ambient air. Therefore, a general convection heat transfer condition is applied to the glass plate surface. The glass plate surface's heat transfer coefficient is 6 W/m² °C, and the ambient air temperature is set to 25 °C. All the wall boundary layers exposed to

fluid are in the no-slip condition. The pyrolysis vessel's initial temperature is 37 °C, which was the air temperature of the experimental pyrolysis vessel when that of the warm water attained 90 °C. The model is calculated transiently. Air, NH₃, and CO₂ are assumed to be ideal gases. The time step of the calculation is 1 min, and the calculation results are summarized every 10 min.



Figure 4. Schematic diagram and boundary definitions of AC sublimation model validation.

3. Results and Discussion

The variations of the shape of AC in the experiment and simulation are compared in Figure 5. In the experiment, the solid AC area decreases gradually owing to sublimation after heat is supplied. In particular, the solid regions adjacent to the fins and side wall (where heat is supplied directly) are reduced substantially. It means that the fin's large contact area with AC enhances the sublimation. Hence, it can be mentioned that the increasing the number of fins is an effective way to ensure a consistent pyrolysis performance when designing an AC reactor. The simulation also show similar results of the rapid sublimation of solid AC around the sidewall and the fins.

The reactor pressures and the gas flow rates of experiment and simulation are compared in Figure 6. In the experiment, the reactor pressure increases to 0.1 bar at 30 min because the exhaust line is closed. After the exhaust valve is opened, it decreases to 0.03–0.04 bar. The flow rate of the exhaust from the reactor decreased from 0.27 l/min at 30 min to 0.05 l/min at 150 min in the experiment. The simulation result of pressures and flow rate show similar changes with experiments. From the Figure 6, it can be said that the developed sublimation model well predicted reactor pressure and the ammonia gas flow rate.



Figure 5. Variation of the shape of solid ammonium carbamate when the reactor is heated.



Figure 6. Pyrolysis reactor (a) pressure and (b) exhaust gas flow rate variation.

The averaged pyrolysis rate was calculated using the above simulation results with 30-min intervals, and is shown in Figure 7. The averaged pyrolysis rate during the first 30 min is 4.32 g/min, and it decreases rapidly to 0.2 g/min. This is because the AC adjacent to the sidewall or fins are sublimated rapidly by conductive heat transfer in the early stage of the experiment. After that, the sublimation rate of the remaining AC is controlled by the heat supplied by convection.



Figure 7. Ammonium carbamate pyrolysis rate variation.

The simulated temperatures are compared with the experimental results in Figure 8. All the temperatures of thermocouples increase linearly by heating initially, and the temperatures are saturated after sublimation has occurred. This means that all energies supplied to the reactor are used as the latent heat of sublimation. The simulation also shows the saturation of temperatures. However, in the experiment, the temperatures are saturated quickly, whereas it takes longer for saturation in the simulation. It seems that this difference comes from the uncertainties of simulation, such as the inexact values of heat capacity or density of solid AC the heat transfer characteristics of porous space in the solid AC may also be affected.

Comparing the temperature distribution of the experiment reveals that TRF3 and TRA2 are the hottest (70–80 °C). It seems that the thermocouples in these regions were rapidly exposed to hot gases because of fast sublimation by a large amount of heat supplied from the sidewall. The temperatures of TRF1 and TRF2 are the second highest (65–72 °C) because these were close to the fin and exposed to the gases after about 90 min. The temperature of TRA1 are the lowest (62–70 °C) because it was farthest from the fin and sidewall. It seems that the thermocouple rod of TRA1 was buried in AC for the entire experiment. Similarly, in the simulation, the temperatures of TRF3 and TRA2 are the highest, and that of TRA1 is the lowest. These are similar with the experiment results.

Generally, the temperature measured in the experiment is high in the order of height. The temperatures are low in the AC or near the AC because the AC absorbs heat during sublimation. However, there is an exceptional temperature distribution in the experiment. For example, the temperature at Point 4 of TRA1 is higher than that at Points 2 and 3 of TRA1 during the entire experiment. Additionally, the temperatures at Point 4 of each TRF1, TRF2, and TRA2 are higher than that at Points 2 and 3 of each TRF1, TRF2, and TRA2 during the first 100 min of the experiment. It seems that the voids in the AC cause an unexpected temperature distribution. The thermocouple exposed to the gases in a void shows a higher temperature than that of the thermocouple buried in AC because of little or no latent heat of AC sublimation. After 100 min, all temperatures of Point 4 were lower than point 2 and point 3. This means that the AC near Point 4 collapsed, and the thermocouples at Point 4 were buried in AC again.



Figure 8. Variation in temperature distribution of (**a**) TRF1, (**b**) TRF2, (**c**) TRF3, (**d**) TRA1, and (**e**) TRA2.

In the simulation, the temperature is high in the order of height without exception. The reason is that the continuous collapse of upper solid AC into the lower space by the effect of gravity was taken into account in the simulation. From the above results, it can be mentioned that it is challenging to accurately predict the spatial temperature distribution in the reactor where AC sublimation occurs because it is necessary to accurately predict the collapse of the solid AC existing in the upper or surrounding area into the lower empty space.

4. Conclusions

In this study, a numerical model for the sublimation of AC is newly developed. To effectively simulate the sublimation of AC in a reactor, the calculation zones are divided into three zones with different characteristics: solid-phase zone, gas-phase zone, and sublimation zone. Depending on the sublimation critical temperature (T_{th}) and the solid-phase and gas-phase mass ratio (ρ_s) in the zone, the solid-phase zone changes to the

sublimation zone and then to the gas-phase zone. This study also simply modeled the collapse of upper solid AC into the lower empty space, which is created by sublimation.

The simulation results were compared with the experimental results of AC sublimation in a simplified reactor. It is found that the modeling can show very credible information about the phenomena of AC sublimation, such as temperature change with time, the reactor pressure, and sublimated gas flow rate. It is also conjectured that the heat transfer in the reactor is reasonably simulated because the shape variation of solid AC in the experiment is similar to that in the simulation. However, the accurate prediction of spatial temperature distribution is challenging because it is related to the accurate prediction concerning the collapse of the solid AC existing in the upper or surrounding area into the lower empty space, caused by sublimation.

Author Contributions: Model development and simulation, J.-H.N., experiment and writing-original draft, S.-H.W., writing-review and editing, H.R., conceptualization, and supervision, H.K. All authors have read and agreed to the published version of the manuscript.

Funding: This research was funded by the Korea Institute of Machinery & Materials, Republic of Korea, under the project name of "The ultra clean machinery technologies of future electric generation or power systems against PM2.5 fine particles and greenhouse gases", grant number NK231A.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Conflicts of Interest: The authors declare no conflict of interest.

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