Numerical analysis of ammonia decomposition and hydrogen conversion system using DC thermal plasma

H.J. Lee[1], S.P. Kang[1] and T.H. Kim[1*]

[1] *Department of Chemical Engineering, Wonkwang University, Iksan 54538, Republic of Korea*

Abstract: The ammonia decomposition and hydrogen conversion process using thermal plasma is very efficient due to the high economic efficiency and eco-friendly process without carbon dioxide. However, it is difficult to observe the detailed decomposition and conversion reactions by extremely high temperature and rapid velocity of the plasma jet. Therefore, the decomposition and conversion reactions were firstly analyzed by calculating theoretically the characteristics of heat flow.

Keywords: Thermal plasma, Numerical analysis, Ammonia decomposition, Hydrogen conversion

1. Introduction

According to the global annual energy usage distribution, fossil fuels are estimated to be about 80%, renewable energy is 14%, and nuclear power is 6% [1]. Greenhouse gases emitted from fossil combustion have a great impact negatively on the environment. Therefore, the use of clean energy is necessary to reduce the increase of greenhouse gases emission. Hydrogen is promising clean energy source that generates water solely as a by-product during combustion [2,3]. However, its storage and transportation are the biggest challenge, currently it was performed through a cryogenic liquefaction method.

The hydrogen fuel has been generally producing by steam reforming, gasification, and partial oxidation methods [4,5]. Since these technologies still spend fossil fuels, total energy consumption and carbon emissions are extremely high. The electrolysis, regard to clean hydrogen production methods, achieve energy efficiency above 70%, but it requires high electricity cost [6].

Compared to former techniques, hydrogen production by ammonia decomposition using the plasma has eco-friendly and cost-reducing advantages. It is able to produce 99.999% pure hydrogen gas at atmospheric pressure in absence of catalyst [5].

In this work, ammonia decomposition and hydrogen conversion system is supposed by thermal plasma enables mass production and rapid conversion time. The extremely high temperature, sharp temperature gradient, and rapid velocity disturb to observe the detailed decomposition and conversion reactions. In order to understand the process, the temperature and velocity distribution of thermal plasma system through numerical simulation, hydrogen production reactions were estimated by thermodynamic equilibrium calculation.

2. Simulation method

A schematic diagram of DC thermal plasma system for ammonia decomposition and hydrogen conversion was indicated in Fig. 1. Non-transferred torch was used, and a reactor was insulated with a castable material.

Fig. 2 shows a simulation domain and mesh of the plasma torch which was applied in this work. The simulation was performed as two-dimensional axi-symmetry. It was calculated governing equations of mass, momentum, and energy conservation, and assumed steady state. And the plasma jet was regarded to be optically thin plasma in the LTE (Local Thermodynamic Equilibrium) state.

To valid the simulation methods and results, the calculated voltage was compared with the measured voltage in experiments. The voltages were presented at Table 1. The flow rate of plasma forming gas was fixed at 50 slpm N_2. Input current was controlled from 20 A to 80 A, input power was varied from 6.3 kW to 18.8 kW.

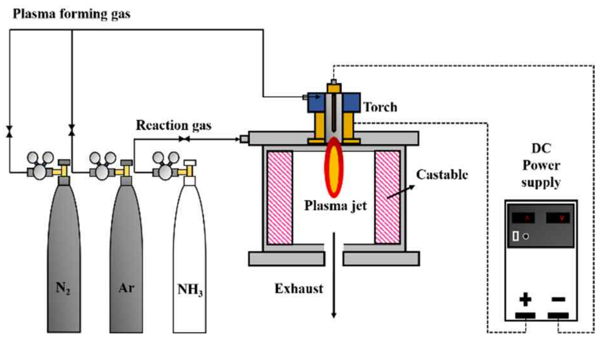

Fig. 1. Schematic diagram of DC thermal plasma system for ammonia decomposition and hydrogen conversion.

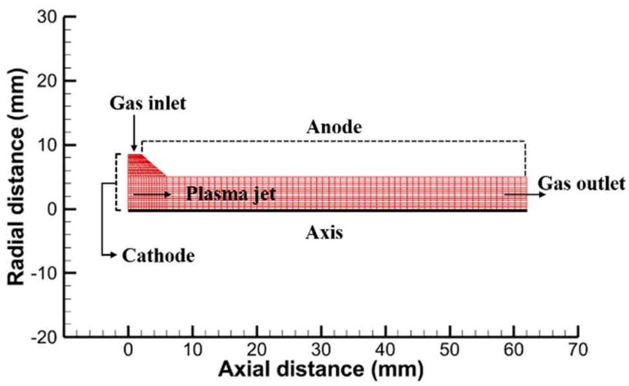

Fig. 2. Simulation domain and mesh of plasma torch.

Table 1. The calculated and measured voltage according to input current.

Plasma forming gas	N_2; 50slpm			
Input Ampere	20 A	40 A	60 A	80 A
Calculated Voltage	171 V	140 V	131 V	126 V
Measured Voltage	315 V	280 V	245 V	235 V

3.Thermodynamic equilibrium calculation

In order to estimate efficient temperature range for ammonia decomposition and hydrogen conversion reactions, thermodynamic equilibrium calculation was performed by HSC Chemistry software (METSO OUTOTEC, ver. 10.1.0.1, Finland). Fig. 3. Indicates the change in Gibbs free energy as a function of temperature for the ammonia decomposition and hydrogen conversion. The reaction for $N_2 + 2NH_3 \rightarrow 2N_2 + 3H_2$ shows a negative value over the entire temperature range. Thermodynamic equilibrium chemical elements were presented in Fig. 4. NH_3 is decomposed into N_2 and H_2 above 500 K, and H_2 is mostly produced in the range of 500 K to 2,500 K.

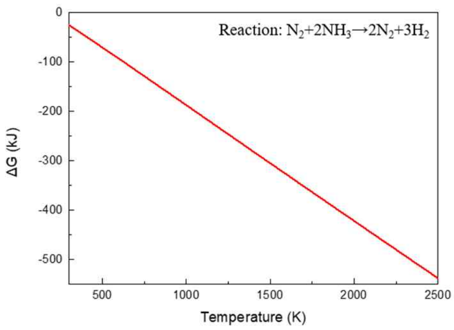

Fig. 3. Change of the Gibs free energy for the ammonia decomposition and hydrogen conversion reaction.

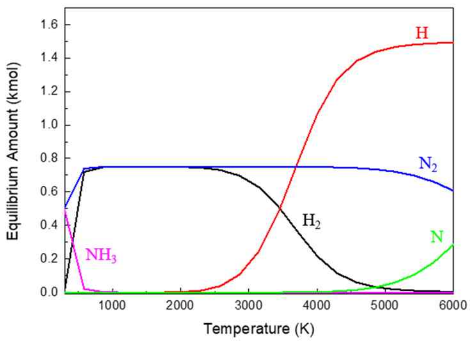

Fig. 4. Thermodynamic equilibrium amount ammonia and nitrogen system.

4.Results and Discussion

Fig. 5 shows temperature distributions inside the torch according to input current for the plasma forming gas N_2 and Ar conditions. As increase the input current, the higher temperature region especially above 7,000 K becomes expanded with the enhancement of input power in both plasma gases. The higher temperature is created by Ar plasma forming gas compared to N_2 gas. And the temperature is rapidly decreased as increasing the radial distance.

Fig. 6. indicates the temperature distribution at the torch exit according to the input current with various plasma forming gases; 50 slpm N_2 and Ar. In N_2 plasma, the highest temperature in 20 A to 80 A is about 6,100 K to 7,100 K. In Ar plasma, the values are about 6,500 K to 9,500 K for 20 to 80 A. The maximum temperature was higher with argon plasma forming gas due to the higher electric conductivity.

These temperature profiles were applied to the computational calculation for the reactor as the boundary conditions. And the thermal flow was analyzed to discuss for the decomposition and conversion reactions which estimated by thermodynamic equilibrium calculation.

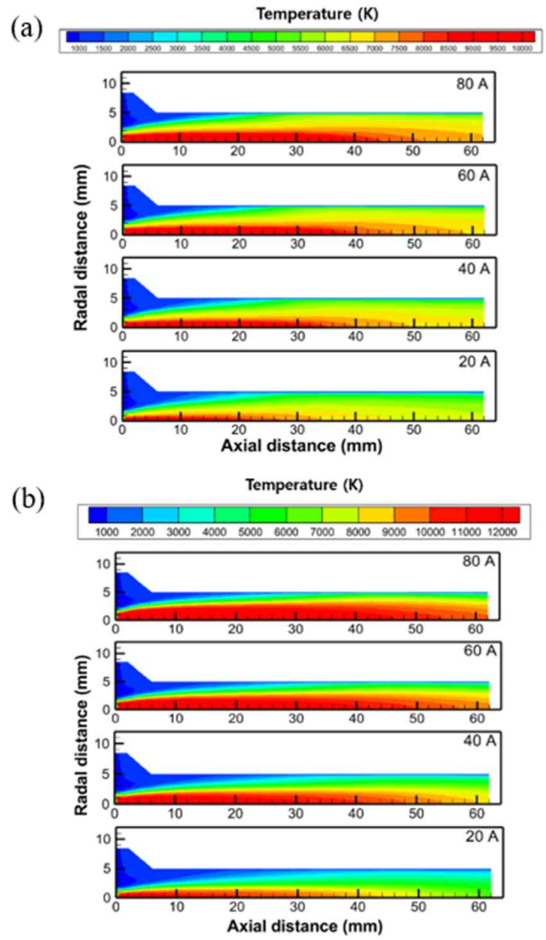

Fig. 5. Temperature profiles inside torch according to the input current. The plasma forming gas was fixed at 50 slpm (a) N_2 and (b) Ar.

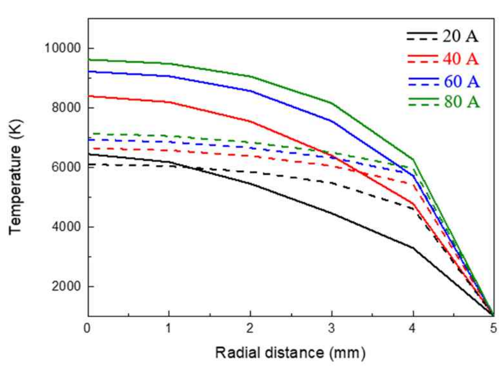

Fig. 6. Temperature profiles at torch exit according to the input current at a flow rate 50 slpm. (dashed lines: N_2, solid lines: Ar)

5.Summary & future plan

Thermal plasma torch was analyzed by the numerical simulation according to the arc voltage and the kinds of plasma forming gas; Nitrogen and argon. The appropriate temperature range of the ammonia decomposition and hydrogen conversion reactions was calculated through thermodynamic equilibrium calculation. In addition, a numerical simulation of the reactor is required to understand the details of process. The ammonia decomposition and hydrogen conversion reactor will be simulated with commercial computational fluid dynamics (ANSYS-FLUENT, ANSYS. Inc, ver. 22.2.0, United Sates). And the calculated optimal condition will be applied for the hydrogen production experiments.

6.References

[1] M.A.K. Lodhi, International Journal of Hydrogen Energy, **29**, 11 (2004).
[2] M. Balat, International Journal of Hydrogen Energy, **33**, 15 (2008).
[3] A. Demirbas, K. Dincer, Energy Sources, Part A: Recovery Utilization and Environmental Effects, **30**, 13 (2008).
[4] L. Barelli, G. Bidini, F. Gallorini, S. Servili, Energy, **33**, 4 (2008).
[5] J.D. Holladay, J. Hu, D.L. King, Y. Wang, Catalysis Today, **139**, 4 (2009).
[6] F. Barbir, Solar Energy, **78**, 5 (2005).