Numerical study on reactor design of methane pyrolysis process using thermal plasma for hydrogen production

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Abstract: Thermal plasma-based methane pyrolysis is one of the methods to produce hydrogen without greenhouse gas emissions. This study numerically analyzed the conversion rate and selectivity according to the change in the linear length and diameter of graphite, and then it presented the optimal conditions. As graphite's length increased, the CH_4 conversion and C_2H_2 selectivity increased by about 10%, and the H_2 selectivity increased by about 6%.

Keywords: Methane pyrolysis, Thermal plasma, Numerical simulation, Graphite linear.

1. Introduction

Methane pyrolysis is one of the methods to produce hydrogen without greenhouse gas emissions like CO_2. The final products in methane pyrolysis are hydrogen and carbon solids. And Methane pyrolysis is based on a chemical process, so it is possible to scale up. In addition, The economic feasibility of hydrogen production can be secured by selling solid carbon obtained as a by-product of the reaction [1]. Therefore, methane pyrolysis is possible to produce hydrogen in large quantities at low cost without emitting greenhouse gas [1,2]. Although the methane pyrolysis reaction has many advantages over existing technologies, the biggest reason for not being commercialized is the high reaction temperature and the deposition of solid carbon.

Methane is a very stable molecule due to the strong C–H bonds and the symmetry of its molecular structure. For these reasons, methane pyrolysis occurs only at temperatures above 1100–1200 °C in the non-catalytic process [3]. Thermal plasma is an ionized thermal fluid generated by a plasma torch in the form of a high-temperature jet flame. This is effective as a heat source for methane pyrolysis. However, it is necessary to improve the energy efficiency of methane pyrolysis using plasma [4].

We installed a graphite linear to mix methane and thermal plasma jets effectively to improve energy efficiency. At the same time, the heat was confined to raise the reaction temperature. The reaction temperature and residence time are the most critical variables in methane pyrolysis [5]. That can be adjusted through the shape change of the graphite linear. However, there is a realistic limit to finding the optimal graphite linear conditions through experiments. Therefore, in this study, the optimal conditions to increase the conversion rate and selectivity were derived through computational analysis. A thermal plasma reactor simulation for methane pyrolysis is performed using DCPTUN code and ANSYS-FLUENT software to optimize the reactor design and operating conditions suitable for hydrogen production and methane conversion efficiency.

2. Numerical model

The computational analysis of the methane pyrolysis system was divided into the torch area and the reactor area, and the computational analysis was performed. Numerical analysis is performed by calculating the torch region using the self-developed thermal plasma analysis code DCPTUN.

The plasma torch conditions are as follows. The discharge gas is N_2, the flow rate is 15 L/min, the current is 200 A, and the voltage is 80 V. Fig. 1 shows the velocity and temperature profiles calculated using the DCPTUN code. This applies to the plasma inlet boundary condition. The calculated voltage was 79.1 V, the measured voltage was 80 V, and the error value was 1.1%, which was a minimal value.

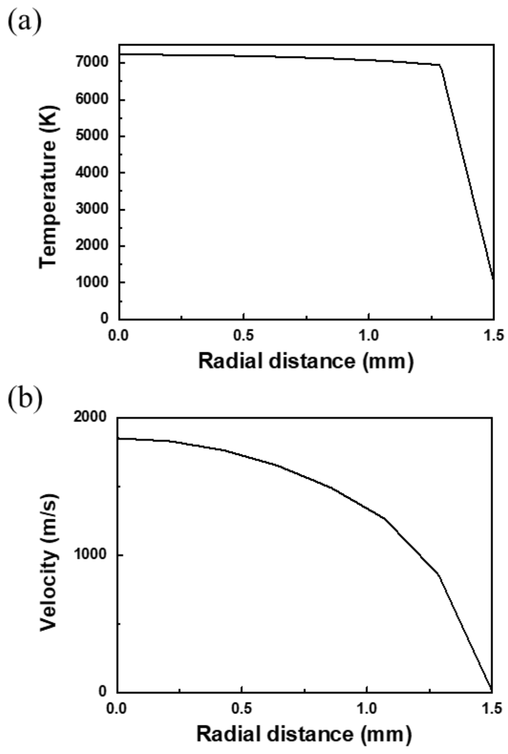

Fig. 1. Distribution of the jet at the exit of the thermal plasma torch calculated by DCPTUN (a) temperature, (b) velocity.

The temperature and velocity of the thermal plasma jet calculated through the DCPTUN code were applied to the plasma inlet boundary condition to calculate the inside of the reactor. Calculations included turbulent flow models(k-epsilon model), radiative heat transfer(P1 radiation model), and chemical reactions to analyze the interaction of CH_4 with the high-temperature thermal plasma jet. The detailed mechanism of methane decomposition from 36 chemical reactions was proposed in [6].

Fig. 2 shows the two-dimensional mesh and boundary conditions for the shape of a single torch methane pyrolysis system for hydrogen production constructed for computational analysis. The thermal plasma torch is installed at the top of the reactor. CH_4 was injected through a hole in the graphite at an axial distance of 0.005 m, which mixed it well with the thermal plasma jet and was used as insulation material to reduce heat loss at the same time, confining the heat, causing a temperature raising effect. The torch input power (16 kW) and methane injection flow rate (10 L/min) were fixed to check the effect of the length and radius of the graphite linear. Computational analysis was performed by varying the inner radius and length of the graphite. The wall boundary of the graphite linear was considered convective conditions at a free stream temperature of 300 K and a heat transfer coefficient of 25 W/m^3-K.

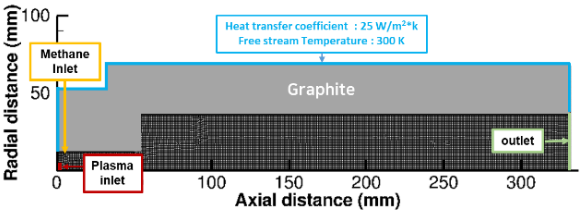

Fig. 2. Schematic of a single plasma reactor for hydrogen production.

3. Result and discussion

Fig. 3 shows the temperature distribution according to the graphite linear length. Methane was injected at an axial distance of 5 mm, and after injection, methane pyrolysis occurred, and it was observed that the temperature distribution was lowered. When the reactor length increased from 332 mm to 432 mm, the temperature at the reactor exit is 1,283 K and 1,117 K, respectively. It decreased by about 100 K. Fig. 4 depicts the mass fraction of CH_4, Fig. 5 is the mass fraction of H_2, and Fig. 6 the mass fraction of C_2H_2. As the graphite linear length increased 332 mm to 432 mm, the mass fraction of CH_4 decreased from 0.1187 to 0.1079, the mass fraction of H_2 increased from 0.0147 to 0.0157, and the mass fraction of C_2H_2 increased from 0.0586 to 0.0599 at the reactor exit. As a result, the CH_4 conversion rate and C_2H_2 selectivity increased by about 10%, and the H_2 selectivity increased by about 6%. This reason is the reaction time increased as the reactor length increased.

As a result of the calculation, the temperature at the outlet is over 1000 K. This confirms that the graphite linear preserves the heat of the thermal plasma well. Moreover, as the reactor length increased, the conversion rate and selectivity increased. It indicates that a chemical reaction occurred at the rear of the reactor. It has been shown that the conversion rate and selectivity increase with increased response time. However, the length of the graphite linear requires proper design. If the graphite linear is too long, conduction heat loss will occur, reducing methane conversion and selectivity.

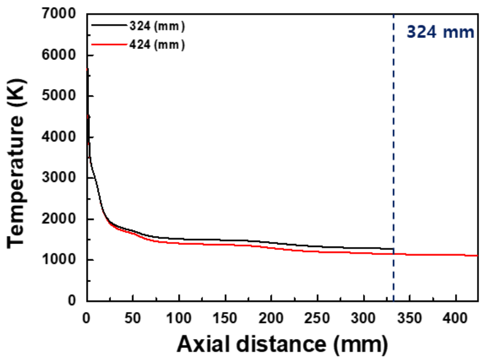

Fig. 3. Temperature distribution in the center of the reactor

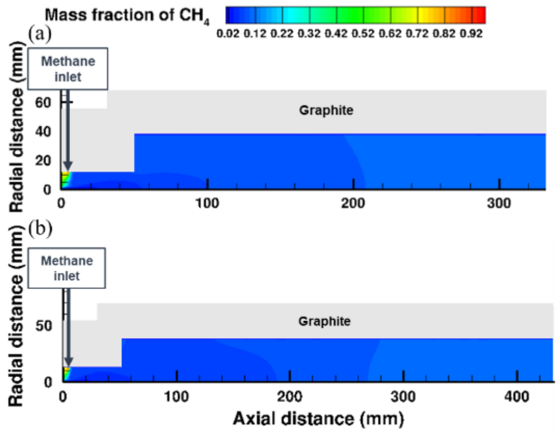

Fig. 4. Mass fraction distribution of CH_4 along the reactor length (a) 332 mm, (b) 432 mm.

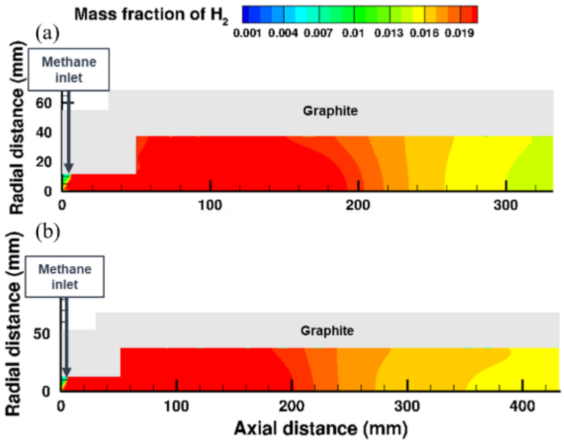

Fig. 5. Mass fraction distribution of H_2 along the reactor length (a) 332 mm, (b) 432 mm.

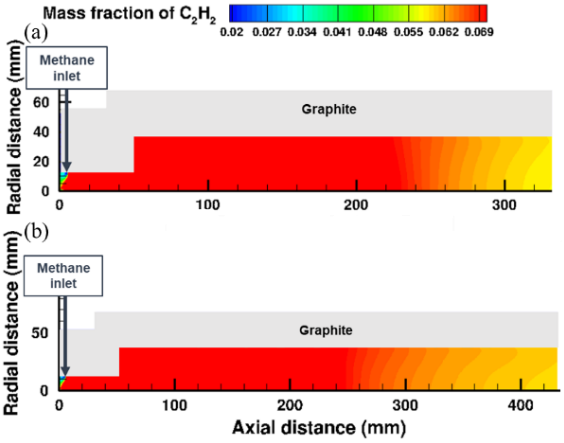

Fig. 6. Mass fraction distribution of C_2H_2 along the reactor length (a) 332 mm, (b) 432 mm.

4. Conclusions

It is possible to confirm through analysis that the change in the length of the graphite linear affects the conversion rate and selectivity due to the increase in reaction time. Therefore, in the future, the length or radius of the graphite linear will be changed, and the conversion rate and selectivity rate trends will be compared to derive the optimal condition of the graphite linear for hydrogen production.

5. References

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