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Design and Simulation of a Novel Copper-Chlorine Thermochemical Cycle for Hydrogen Production

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I. Introduction

Thermochemical cycles are one of the hydrogen production techniques that involves splitting water into oxygen and hydrogen by Khalid (2016). In the cycle, serial reactions take place to split water into oxygen and hydrogen. Each reaction represents a reaction step. While many thermochemical cycles require temperature of more than 800℃, the maximum temperature required for the Cu-Cl cycle is 550 ℃ by Farsi (2020). . Configuration of the Cu-Cl thermochemical cycle varies depending on the number of steps and the type of reaction occurring within the cycle by Sattler (2017). Many studies presented in the literature include an electrochemical step in addition to chemical reactions. Due to increasing electricity prices and the expense of the electrolysis equipment used, studies are being carried out to reduce or eliminate the electrical load brought on by the electrolysis step.

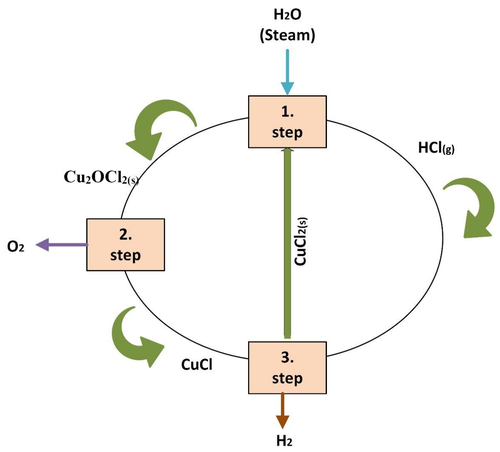

Figure 1. Simplified demonstration of the proposed 3-step Cu-Cl cycle

II. Objectives

- To improve and evaluate a new Cu-Cl thermochemical cycle.
- To find a new reaction that works entirely thermally instead of an electrolyzer.
- To evaluate the new reaction, simulations are created using Aspen Plus.

III. System Description

The Cu-Cl cycle begins with the hydrolysis of $CuCl_2$, and after the decomposition of Cu_2OCl_2, the production of hydrogen completes the cycle. Within the cycle, the following reactions occur:

- Hydrolysis step (Step 1):

$2CuCl_{2(s)} + H_2O_{(g)} \longrightarrow Cu_2OCl_{2(s)} + 2HCl_{(g)}$ (T=400 ℃)

- Thermolysis step (Step 2):

$Cu_2OCl_{2(s)} \longrightarrow 1/2O_{2(g)} + 2CuCl_{(l)}$ (T=530 ℃)

- Hydrogen production step (Step 3):

$2CuCl + 2HCl_{(g)} \longrightarrow 2CuCl_{2(s)} + H_{2(g)}$ (T=500 ℃)

IV. Method and Analysis

Aspen Plus simulations of the 3-step Cu-Cl cycle have been performed in this study. The Figure 2 shows the Aspen plus flowsheet of the 3-step Cu-Cl thermochemical cycle. The reactors used in the system simulation are RStoic reactors, while the selected method is the is the solid method in the Aspen Plus.

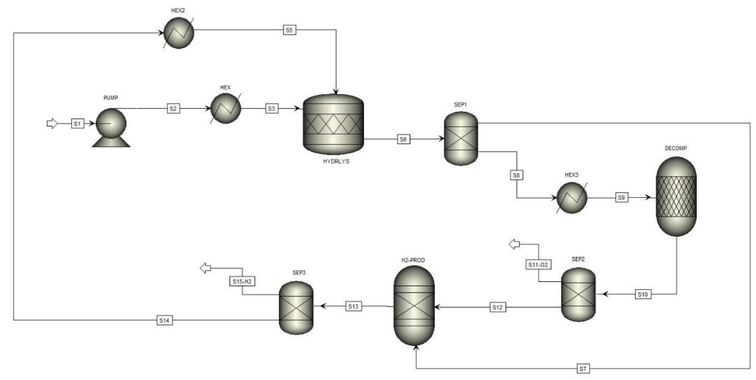

Figure 2. Aspen plus flowsheet of the 3-step Cu-Cl thermochemical cycle

V. Results

After the system simulation using Aspen Plus, by increasing the molar flow rates of water fed to the hydrolysis reactor from 3000 kmol/h to 5000 kmol/h, the effect of the produced Cu_2OCl_2 molar flow rate and the heat duty of the first heat exchanger is analyzed by performing a parametric study. Figure 3a shows that effect of H_2O mol flow rate on the produced Cu_2OCl_2 and heat duty of HEX1. Figure 3b shows the effect of $CuCl_2$ mol flow rate on the produced H_2 and heat duty of HEX2.

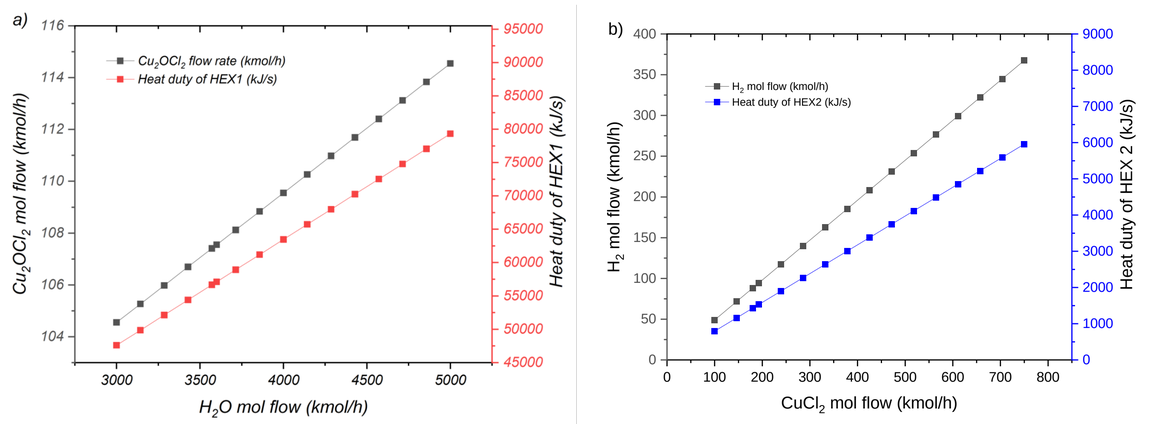

Fig. 3: a) the effect of H_2O mol flow rate on the produced Cu_2OCl_2 and heat duty of HEX1, b) the effect of $CuCl_2$ mol flow rate on the produced H_2 and heat duty of HEX2.

VI. Conclusion

As a result of the parametric studies conducted, with the increasing mole flow rate of reactants, the amount of heat duty to be provided to the heaters used in the system also increases. For this reason, the optimum flow rate of the reactants should be determined. As a result of 0.05 kmol/s $CuCl_2$ and 1 kmol/s H_2O reactant input into the system, the H_2 molar flow rate produced by the system was found to be 0.0245 kmol/s.

References

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