Life cycle assessment of hydrogen production from waste-derived ammonia decomposition using metal catalysts

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ABSTRACT - Hydrogen is as an energy source with clean combustion. Conventional hydrogen production technologies from hydrocarbons could have carbon emissions in the fuel cells. Ammonia decomposition can be considered as a carbon-free method of hydrogen production. The objective of this study is to conduct a comparative life cycle assessment for scaled-up hydrogen production from waste-derived ammonia decomposition on Ru/Al_2O_3 and Ni/Al_2O_3 catalysts. The hydrogen production processes were scaled up using the process simulation technique. The simulated process data for both catalyst routes were applied to evaluate the net energy analysis and global warming potentials at the same unit basis. According to the obtained results, Ru/Al_2O_3 has the highest net energy indicators than the Ni/Al_2O_3. The conventional air stripping method for waste-derived ammonia production has a negative net energy value compared to the Microbial Fuel Cell (MFC) process. Global Warming Potential (GWP) was calculated for both catalysts routes and the results show that both processes have close GWP values.

Key words: Hydrogen production; Ammonia decomposition; Life cycle assessment; Process Simulation

INTRODUCTION

Conventional fossil fuel burning increases greenhouse gas emissions causing climatic changes like global warming. Hydrogen is a clean energy source with water as the only by-product from combustion. Fuel cell is a promising technology to produce electrical energy using H_2 retrieved from another source and O_2 as fuel because it offers higher energy conversion efficiency (Vaidya et al., 2006). Hence, there is a growing interest about using fuel cells to produce electricity for mobile and stationary applications. Conventional hydrogen production technologies from hydrocarbons could incur carbon emissions in the fuel cells. However, hydrogen can be produced with carbon-free environment from ammonia decomposition. Metal catalysts could be used to increase the reaction rate of ammonia decomposition (Bell & Torrente-Murciano, 2016)

METHODOLOGY

Process Simulation Method

The process simulations to scale-up ammonia decomposition process was conducted using Aspen Plus software as the process simulation tool. Two separate large-scale plants were simulated for Ru, and Ni catalysts with Al_2O_3 support in the packed bed reactor. Ammonia was recovered from wastewater containing urine was either from Conventional Air Stripping or Microbial Fuel Cell (MFC) process.

Simulation Procedure

The reaction rate is given by Temkin–Phyzev mechanism as in Equation (1) (Chellappa et al., 2002).

$$r = k_o exp(\frac{-E}{RT}) \times (\frac{P_{NH_3}^2}{P_{H_2}^3})^{\beta} \quad (1)$$

Large-scale operating conditions are far different from the experimental scale at the laboratory. Therefore, reaction kinetics were adjusted based on simulation results as shown in Table 1.

Life Cycle Assessment

Life cycle assessment was conducted according to the ISO 14040/44 framework as the LCA methodology.

Goal and Scope

Selected functional unit is 1,000 kg of hydrogen production from ammonia decomposition process. The defined system boundary (SB) extends to ammonia recovery from wastewater containing urine by the sated two methods, and catalyst/support extraction phase to the hydrogen storage stage.

Inventory Analysis

This study utilizes mainly the following literature-based assumptions for calculations/simulations.

1. Approximately 95% urine stored in wastewater is hydrolysed to ammonia. Ammonia removal efficiency is 83.5% at 30 ˚C.
2. Net energy analysis is done for 60% NH_3 conversion for both Ru/ Al_2O_3, Ni/Al_2O_3.

Based on inventory data energy consumptions/generations are calculated for both plants. In the net energy analysis, Net Energy Value (NEV), Net Renewable Energy Value (NRnEV), Net Energy Ratio (NER), and Renewability indicators were calculated.

Net energy value = total net energy outputs - total net energy inputs (2)

$$Net\ energy\ ratio = \frac{net\ energy\ outputs}{net\ energy\ inputs} \quad (3)$$

$$Renewability = \frac{net\ energy\ outputs}{net\ fossil\ energy\ inputs} \quad (4)$$

Impact Assessment

In this study, gas emission analysis and Global Warming Potential (GWP) impact are evaluated for the 3 process stages: raw material stage, transportation stage, and manufacturing stage, including hydrogen storage stage.

Table 1. Reaction kinetics from simulation model

Parameter	**Ru/Al$_2$O$_3$**		**Ni/Al$_2$O$_3$**	
	Laboratory scale	Simulation model	Laboratory scale	Simulation model
k_o (mol-NH$_3$/Ni^0 s Pa^b)	3.75×10^{13}	7.50×10^{8}	3.16×10^{5}	7.50×10^{4}
E (kJ/mol)	117	160.5	102	140.3
B	0.5	0.6	0.2	0.3
Reference	(Chiuta et al., 2016)	From this study simulation	(Zhang et al., 2005)	From this study simulation

$$Climate\ change = GWP_{100,i} \times m_i \qquad (5)$$

Where, $GWP_{100,i}$= global warming potential over 100 years of substance.

RESULTS AND DISCUSSION

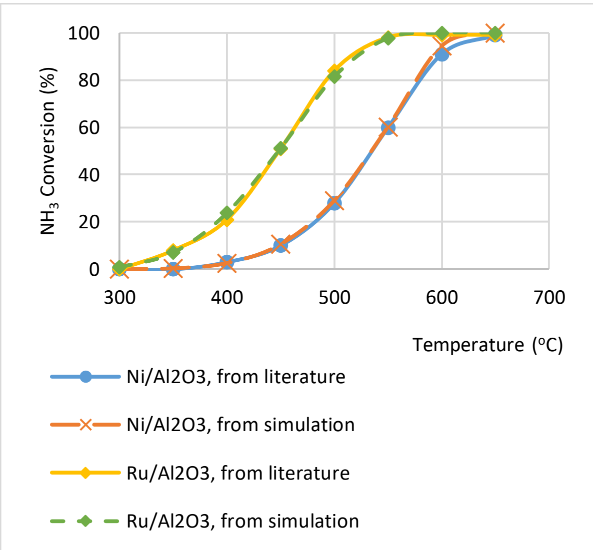

Figure 1. Comparison of simulation results of ammonia conversion over Ru/Al$_2$O$_3$ and Ni/Al$_2$O$_3$ in this study with published experimental results

According to the results for reaction kinetics for the simulation model, the packed bed reactor was simulated for both catalysts at the same temperature range. It is obvious that Ru/Al$_2$O$_3$ gives higher conversion than Ni/Al$_2$O$_3$ at the same temperature. Simulation results are validated by using the published experimental results (Figure 1). For both scenarios, net energy indicators are evaluated. When Ru/Al$_2$O$_3$ is used as the catalyst, the net energy value is 35,121 MJ/FU. Also, the net energy ratio is 1.22 and renewability is 63.34. For the Ni/Al$_2$O$_3$ net energy value is 17,372MJ/FU, net energy ratio is 1.1 and renewability is 63.34. Therefore, Ru/Al$_2$O$_3$ has the highest net energy value due to its catalytic activity.

Also, environmental emission analysis is performed for both scenarios, phase by phase. It shows the carbon emission is higher in the electricity generation phase and transportation phase for both scenarios. SO_2 emission is higher in Ni/Al$_2$O$_3$ production phase while CO_2 emission takes first place in Ru/Al$_2$O$_3$ production. However, global warming potential (GWP) for the two scenarios of catalysts are very close to each other.

CONCLUSION

According to the results from net energy analysis, Ru is a lower energy consuming catalyst, compared with Ni for the hydrogen production life cycle from ammonia decomposition, because the ammonia decomposition process using Ru catalyst has a higher net energy value and net energy ratio than the Ni involved process. But the process which uses Ni as the catalyst, which has a close global warming potential to the process using Ru could be used as an alternative process. Future investigations can be performed to evaluate other environmental impacts of the two processes, including production and environmental cost analysis. This study can support the selection of more environmentally-benign catalyst for hydrogen production by decomposition of ammonia, derived from waste sources.

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