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Comparative Techno-economic Assessment of Hydrogen Production, Storage and Refueling Pathways

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ABSTRACT

Hydrogen, as a clean and versatile energy carrier, holds immense promise for addressing the world's growing energy and environmental challenges. However, hydrogen-based energy systems face challenges related to efficient storage methods, energy-intensive production, refueling processes, and overall cost-effectiveness. To solve this problem, a superstructure was developed that integrates overall technologies related to hydrogen energy transportation. This study synthesizes process pathways for hydrogen energy transportation method including energy carrier production, storage, and refueling, based on the developed superstructure. The techno-economic analysis was conducted to evaluate the performance of each transportation pathway and compare it with conventional fossil fuel transportation system. Process performance criteria, including unit production cost (UPC), energy efficiency (EEF), and net CO₂ equivalent emissions (NCE), serve as indicators for process performance. By comparing technological pathways, we can propose the most economically and environmentally optimal energy refueling route. Additionally, sensitivity analyses were performed on various external factors, identifying influential variables in the decision-making process for hydrogen production, storage, and refueling strategies, while also elucidating technological limitations.

Keywords: Hydrogen, Process synthesis, Environment, Techno-economic analysis, Energy refueling

1. INTRODUCTION

One of the most important global environmental issues is the depletion of conventional energy sources and the climate change caused by greenhouse gas (GHG) emissions. Hydrogen is flexible energy carrier that can be converted into usable forms of energy and is an environmentally clean energy source. The concept of hydrogen economy, characterized by the production, distribution, and utilization of hydrogen as a primary energy carrier, has gained significant traction. The transformative vision envisions a departure from conventional fossil fuel dependency toward a circular and interconnected energy system where hydrogen acts as a linchpin for integration, storage, and efficient utilization of renewable energy sources.

To establish a hydrogen energy system, various preliminary studies are being conducted on developing hydrogen production, storage, and transportation systems. Li Lin et al. conducted the process development and cost analysis of an ammonia-based hydrogen refueling station process [1]. A.D. Korberg et al. developed and evaluated a transport process for renewable energy resources [2]. Jack Shepherd et al. developed a green ammonia value chain and proposed the pathway with the highest economic feasibility [3]. Ayodeji Okunlola et al. proposed an optimal hydrogen transportation method through analysis of inter-country hydrogen transportation and supply [4].

In preliminary research, the development of technologies for the production, storage, and transportation of hydrogen is progressing, and research on establishing hydrogen energy system is also being conducted. However, the previous study has not determined and evaluated compared conventional fossil fuel transportation system. We compared and analyzed the energy system, including hydrogen production, storage, and transportation, with the conventional fossil fuel-based energy system to determine the possibility of hydrogen replacing conventional energy resources. This study focused on



various hydrogen storage and transportation method such as high-pressure compression, liquefaction, ammonia, liquid organic hydrogen carriers (LOHC). Each developed hydrogen storage and transportation method is synthesized with a process for production hydrogen form various energy sources.

This study developed the superstructure of the entire energy transfer based on hydrogen and fossil fuels. An energy transport pathway was developed by modeling various unit processes within the superstructure. Then, a techno-economic analysis is performed for each pathway to derive energy efficiency (EEF), levelized cost of energy (LOCE), and net CO_2 equivalent emissions (NCE), which are quantitative indicators of process performance. Through the results of techno-economic analysis, a process pathway with optimal economic or environmental feasibility for hydrogen energy transportation was derived. In addition, we identified technical limitations for establishing a hydrogen energy system and proposed technical and political strategies.

2. RESEARCH OVERVIEW AND METHODOLOGY

Research Overview

The goals of this work are: i) to propose optimal economic or environmental hydrogen energy transportation pathway, ii) to determine technical limitation of hydrogen energy transportation system, iii) to propose technical and political strategies for hydrogen energy system. Figure 1 provides procedures for energy transportation system development. First, we set problem by investigating energy sources, conversion technologies, and energy carriers and making a database of the technical and social data. To identify the overall structure of the hydrogen energy transportation system, a superstructure connecting transportation technologies was developed based on technical data. Then, a unit process model on the energy transportation system superstructure was developed and the mass and energy balance for each energy transport pathway was derived through process synthesis. Through a techno-economic analysis of each developed process model, process efficiency, cost, and CO₂ emissions are calculated.

Primary energy source considered in this study include conventional fossil fuels such as coal, crude oil, and natural gas, as well as renewable energy sources such as wind energy, solar energy, and biomass. These energy sources can be transported as is or converted into other forms of energy carriers. Table 1 shows information on the energy carriers considered in this study. The energy carriers considered in this study of fossil fuels transported as primary energy sources, hydrogen for transporting renewable energy, and hydrogen carriers for efficient transport of hydrogen. Among them, hydrogen is the most important material and serves as an intermediate for transportation with high energy density. However, hydrogen has a low density, making it difficult to transport. Therefore, convertible materials were considered to facilitate transportation of hydrogen from energy resources: ammonia, methanol, methyl cyclohexane (MCH), perhydro dibenzyl toluene (H₁₈-DBT).

Table 1: Energy carrier for hydrogen transportation system.

Transportable primary energy source	
Coal	
Crude oil	
Natural gas	
Biomass	
Converted energy carrier	Description
Hydrogen	H_2
Methanol	CH₃OH
Ammonia	NH ₃
Methyl cyclohexane	C ₇ H ₁₄
H ₁₈ -Dibenzyl toluene	C ₂₁ H ₃₈

Process Analysis Method

In this study, the techno-economic and environmental feasibility was evaluated using the process

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performance indicators such as EEF, LCOE and NCE.

To determine technical aspects of hydrogen energy transportation pathways, EEF serves as an assessment indicator. EEF is expressed as the ratio of transported energy to the total of primary energy and utility consumption for conversion, as shown in Eq (1).

$$EEF = \frac{Transported \, Energy}{Primary \, energy \, source + E_{utilities}} \times 100 \, (\%)$$
(1)

To compare economic performance of the hydrogen energy transportation pathways, the LCOE was used as an indicator. The LCOE is calculated using annualized capital investment (ACI) and total operating cost (TOC) and transported energy as shown in Eq (2).

$$LCOE(\frac{\$}{kWh}) = \frac{ACI+TOC}{Transported energy}$$
 (2)

ACI is an amortized cost of the capital expenditure (CAPEX), which is specified using a straightforward depreciation method, as shown in Eq. (3). The TOC consists of the primary energy source and utility cost which is specified Eq. (4).

$$ACI = CAPEX \times \frac{interes \ rate \ (1+interestrate)^{lifetime}}{(1+interestrate)^{lifetime} - 1}$$
(3)

TOC = Raw material cost + Utility cost (4)

To assess the environmental performance of the



Figure 2: Superstructure of fossil fuel-based and renewable energy transportaton system, NG: natural gas, MCH: methyl cyclohexane, H₁₈-DBT: perhydro dibenzyl toluene, SYN.: synthesis process, DEHYD.: dehydrogenation process [5-10].

hydrogen energy transportation pathways, the NCE was calculated by including two different indicators to CO_2 emissions. First, the direct emission was GHGs (CO_2 , CH_4) that are emitted directly through the exhaust and tail gas during process operation. The second is indirect emissions from the usage of utilities, during the process. Thus, the NCE as an environmental indicator is expressed as the total CO2 emission per transported energy, as shown in Eq. (5).

$$NCE = \frac{Direct \ emission+Indirect \ emission \ (kg \ CO_{2-eq})}{Transported \ energy}$$
(5)

3. RESULT AND DISCUSSION

Superstructure Development

As mentioned above, this study developed superstructure for energy transportation method. We developed two hydrogen energy transportation systems, illustrated in Fig 2: fossil fuel-based energy transportation system, renewable energy transportation system. In the case of fossil fuel-based hydrogen transportation systems, both direct transportation primary energy source and transportation via hydrogen are viable options. The pathway that converts fossil fuels into hydrogen and transport will benefit in terms of transport mass due to the high energy density of hydrogen and is expected to have better environmental performance by using the CO₂ capture process. Hydrogen-based energy carriers are essential to transport renewable energy. There are two reasons for this: the form of energy generated from wind or solar energy is electricity, and the low energy density of biomass.

In this study, a technical information investigation was conducted based on the developed superstructure to build a database. It is used for process simulation and techno-economic analysis through investigation of the operating conditions, raw material prices, and energy consumption of each unit process.

Process Development

In this study, we developed hydrogen production, storage and refueling process models were developed using Aspen Plus V12.0 according to hydrogen transportation superstructure. The information of each unit process is summarized in Table 2. It was assumed that each pathway feeds the same amount of energy based on the primary energy source.

The hydrogen transport pathway was modeled through synthesis between each unit process, mass and energy balance were derived. In addition, a techno-economic analysis is performed using process equipment sizing and costing data within Aspen Economic Analyzer based on mass and energy balance. In the separation and purification technologies, the pressure swing adsorption (PSA) amine-based CO₂ capture process, distillation column and air separation unit (ASU) are mainly adopted for efficient each hydrogen transportation pathway.

Table 2: Unit process information for hydrogen energy transportation pathways [5-11].

Unit process	Operating conditions
	(°C, bar)
Coal gasification	700-1200, 30
Natural gas reforming	700-900, 1
Water gas shift	170-350, 1
CO ₂ capture process	40, 1
H ₂ liquefaction	-253, 20
Liquid H ₂ vaporization	40, 30
NH₃ synthesis	300-350, 100-350
NH₃ dehydrogenation	500, 1
Methanol synthesis	220-250, 50
Methanol dehydrogenation	420, 1
MCH synthesis	210-280, 20
MCH dehydrogenation	320, 1
H ₁₈ -DBT synthesis	150-270, 50
H ₁₈ -DBT dehydrogenation	310, 1
Biomass gasification	450-800, 1

Comparative Analysis

Based on the technical, economic, and environmental parameters derived from the previous process simulation part, a techno-economic analysis was performed to compare and evaluate each hydrogen transportation pathway. As expected, the conventional system for directly transporting fossil fuels has the best efficiency and economic performance for obtaining electricity and thermal energy. The pathway with the economic feasibility compared to these direct fossil fuel transportation methods is natural gas-based hydrogen production and transportation through MCH (0.15 \$/GJ). Hydrogen production using natural gas is currently a representative method of producing hydrogen at the lowest cost, and the MCH hydrogen storage process also shows the best indicator for cost-effective hydrogen transportation with low energy consumption. Additionally, the pathway from an environmental perspective is to produce hydrogen from solar and wind electricity and then transport the hydrogen using H₁₈-DBT. Although this has low economic feasibility due to the price of raw materials, it has the best performance among hydrogen transportation methods in terms of energy consumption, showing the lowest value in terms of NCE due to less use of additional utilities.

4. CONCLUSIONS

In this study, we proposed of most economic or environmental pathways in hydrogen energy transportation systems using it for process performance criteria: LCOE and NCE. This was achieved through process synthesis and evaluation based on hydrogen energy transportation superstructure, and the effect on the application of the hydrogen energy system was shown. The major findings from this study as follows:

To derive the optimal hydrogen energy

transportation pathway according to evaluation standard, process synthesis for energy transport is performed to derive mass and energy balance.

- We conducted techno-economic analysis and derived cost-effective hydrogen transportation method as natural gas-based hydrogen transport to MCH.
- The environmentally best transportation pathway was found to be transporting renewable electricity-based hydrogen as H₁₈-DBT.

In summary, we identified the hydrogen transportation pathway using organic compound is promising energy transportation pathways. As future work, we will expand the scope of energy transportation technologically, geographically, and policy-wise. In addition, we will derive major cost drivers of energy transportation through sensitivity analysis after the development of the energy transportation system and propose energy transportation system strategies through various scenario-based analysis.

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