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Techno-Economic Evaluation and Synthesis of Green Hydrogen Supply Chain with Ammonia as Energy Carrier

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To achieve carbon neutrality by 2050, Malaysian government has identified green hydrogen (H_2) as one of the potential energy sources. However, the high production cost of green H_2 and technical complications of H_2 storage conditions for distribution undermines the strategic framework of the H_2 roadmap in Malaysia. The lack of investments in pre-requisite support infrastructure for the H_2 production, conversion, and storage technologies impedes the progress of the H_2 economy in Malaysia. Recently, ammonia (NH_3) has emerged as a promising carbon-free energy carrier due to its increased ease and safety during transportation and storage. There is limited literature regarding the inclusion of an NH_3 synthesis and storage loop in green H_2 supply chains. This research proposes a systematic approach for the techno-economic evaluation of green H_2 supply chains with green NH_3 as a clean energy carrier of H_2 storage and distribution. A superstructure-based mathematical optimisation model was developed to synthesise the optimum supply chain network configuration for a given optimisation objective. A case study is solved to illustrate the proposed model.

1. Introduction

Malaysia is committed to becoming carbon-neutral by 2050, as highlighted in the 12th Malaysia Plan (Economic Planning Unit, 2021). Therefore, energy-intensive industries are prioritising the reduction of carbon emissions by considering alternative energy sources to fossil fuels. For example, the transport sector is one of top Malaysia's energy consumption sectors in the last decade, accounting for 38 % of the national final energy consumption (Suruhanjaya Tenaga, 2019). As a strategic effort, the Malaysian government has identified H_2, which produces from renewable energy sources, known as green hydrogen (H_2), as one of the potential energy carriers. One of the states in Malaysia, Sarawak launched its first integrated H_2 production plant and refuelling station in 2019, which supports up to five fuel cell buses and 10 fuel cell cars daily (Lim, 2019). The transition towards a H_2 economy also aligns with the United Nations Sustainable Development Goals (SDG) 7—Affordable and Green Energy.

As presented in the literature (Palma et al., 2018), H_2 can be produced from both fossil resources and renewable resources. However, approximately 95 % of global H_2 production still uses the steam methane reforming of natural gas (Brun and Allison, 2022). To produce green H_2, new technologies are required to be implemented and scaled up. Generally, green H_2 costs four times the price of fossil fuel-produced H_2. Additionally, high costs are associated with liquefying or compressing H_2 for storage due to its high-power requirements (Mori and Hirose, 2009) as compared with fossil fuels (e.g., natural gas, gasoline, diesel, etc.). In particular, compressed H_2 gas storage may escalate to 700 bar to compensate for its low volumetric energy density in its ambient gaseous state. Its ease of leaking as a gaseous fuel with a broad flammability range poses a significant safety

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risk (Andersson and Grönkvist, 2019). To overcome the abovementioned challenges to using H_2 as an energy source, a number of research works have been developed. For example, Mah et al. (2020) presented a holistic optimisation model that exploits the use of H_2 for vehicle fueling and electricity generation.

To transform H_2 into a feasible energy source, an alternative carrier in energy storage and distribution systems is needed. Recently, green ammonia (NH_3) is found to be a promising solution, whereby the final H_2 product is converted to and dispatched on-demand as NH_3 before being converted back into H_2 for local consumption at locations with low renewable energy intensity (Kojima, 2019). Since liquid NH_3 consists of higher volumetric energy density, the transportation of energy stored as liquid NH_3 is more cost-effective. There is also a vast existing NH_3 infrastructure due to the widespread use of NH_3 fertiliser within the agriculture sector, and the infrastructure currently being used for propane may also be adopted for liquid NH_3 storage (Valera-Medina et al., 2018).

As NH_3 exists as a gas under atmospheric conditions, its pressure is increased to 9.9 bar for storage in a liquid phase. However, its storage condition is relatively mild compared to the gaseous H_2 storage pressure of 700 bar (Makepeace et al., 2019). Nevertheless, there is still a distinct lack of feasibility studies regarding the commercial scalability of H_2 and NH_3 supply chains in Malaysia.

To address the current limitations, this study aims first to develop a superstructure-based mathematical optimisation model based on a green H_2 supply chain, which also considers an NH_3 synthesis and storage loop for H_2 distribution. This model will then serve as the basis for a techno-economic feasibility analysis for the commercial implementation of NH_3 as an energy carrier for green H_2 supply chains in Malaysia.

2. Methodology

2.1 Supply chain superstructure development

A superstructure model, which considers all possible and alternative processes, technologies and pathways, is first developed. Based on the model, mathematical formulation based on mass and energy balances can be constructed to simulate the behaviour of the green H_2 supply chain. Based on the collected industrial data, Figure 1 shows one of the possible network design configurations whereby palm oil mill effluent undergoes dark fermentation to produce H_2. The raw H_2 gas produced is purified via cryogenic separation before being converted to liquid NH_3 to be stored. The biomethane gas from the first purification unit and the carbon monoxide gas from the second purification unit undergo additional steam methane reforming and water gas shift conversion to enhance the final H_2 yield.

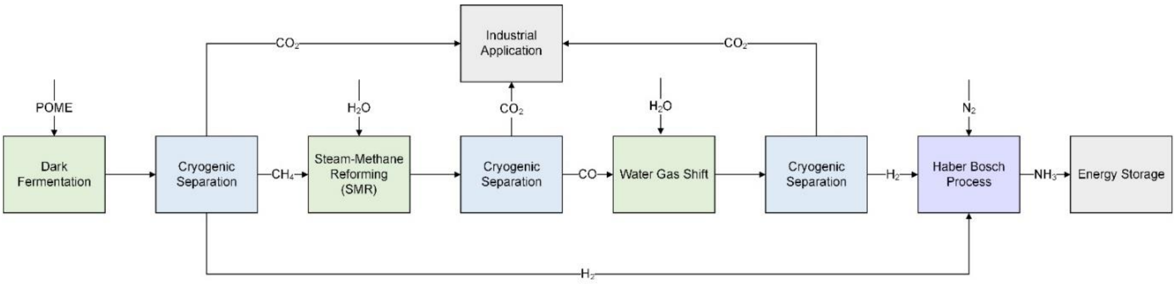

Figure 1: Block flow diagram of an alternative H_2 supply chain configuration

2.2 Model formulation

As mentioned previously, multiple technologies are considered in the synthesis of the green H_2 supply chain (Figure 2). Each technology has its own specifications regarding feed requirements, product conversions, energy consumption and costs. Detailed information on each technology considered in this work is presented in the case study.

Feed *a* enters technology *b,* which converts biomass into intermediate product *c* (H_2) with different purity. The conversion factor of the selection technology *b* is given as x_{abc}. The intermediate product *c* subsequently enters technology *d* to purify intermediate *c* with a conversion of x_{cde} to produce the final product *e* to meet the demand. By drawing a boundary layer with the available feed entering the technology and the utility required to run the technology, the material balance of the intermediate and final components produced by each technology chosen can be determined. The total flowrate of the intermediate product (F_c) and the final product (F_e) can be determined via Eq(1) and Eq(2).

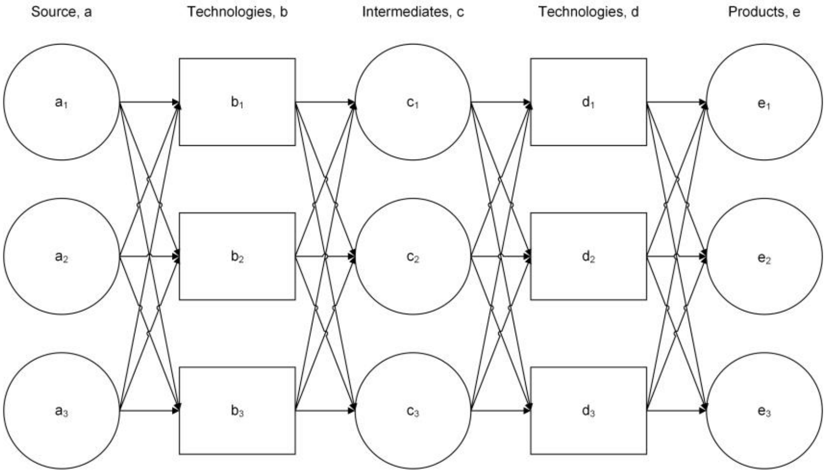

Figure 2: Block flow diagram of an alternative H_2 supply chain configuration

$$F_c = \sum_{b=1}^{B} \sum_{a=1}^{A} F_{ac} \times x_{abc} \tag{1}$$

$$F_e = \sum_{d=1}^{D} \sum_{c=1}^{C} F_c \times x_{cde} \tag{2}$$

whereby F_{ac} represents the flow rate of feed a, x_{abc} represents the conversion factor of technology b and x_{cde} represents the conversion factor of technology d. The energy consumption, EN_b and cost, $COST_b$ associated with technology b are represented in Eq(3) and Eq(4). Likewise, the energy consumption, EN_d and cost, $COST_d$ associated with technology d are shown in Eq(5) and Eq(6).

$$EN_b = F_c \times e_{abc} \tag{3}$$

$$Cost_b = (F_c \times \mathrm{CAPEX}_b \times z_b) + (F_c \times \mathrm{OPEX}_b \times \text{annual attainment}) \tag{4}$$

$$EN_d = F_e \times e_{cde} \tag{5}$$

$$Cost_d = (F_e \times \mathrm{CAPEX}_d \times z_d) + (F_e \times \mathrm{OPEX}_d \times \text{annual attainment}) \tag{6}$$

whereby e_{abc} denotes the energy consumption factor of technology b, CAPEX_b denotes the capital cost of technology b, z_b denotes the number of units of technology b required and OPEX_b denotes the operating cost of technology b. Similarly, e_{cde} denotes the energy consumption factor of technology d, CAPEX_d denotes the capital cost of technology d, z_d denotes the number of units of technology d required and OPEX_d denotes the operating cost of technology d. The annual total cost of the supply chain can be determined by the summation of the total equipment costs and respective utility cost as shown in Eq(7).

$$\text{Minimise} \sum_{b=1}^{B} Cost_b + \sum_{d=1}^{D} Cost_d \tag{7}$$

The optimisation objective is set as the minimisation of annual total costs to synthesise a green H_2 supply chain with maximum economic performance.

3. Case study

Since the Sarawak Economic Development Corporation has begun its initiative of providing free shuttle services via H_2 fuel cell vehicles since last year (Wong, 2022) and the majority of Malaysian H_2 research efforts are concentrated in Sarawak (Mah et al., 2019), the model is applied to an industrial plant in one of the twelve Sarawakian districts.

During the early transition phase from gasoline engines in conventional cars to H_2-powered vehicles, each district is projected to have an average annual H_2 demand of 137 GWh to support a fleet of 10 fuel cell vehicles with a fuel economy of 0.55 kg H_2/100 km (Toyota Europe Newsroom, 2021) based on the annual average vehicle mileage in Sarawak (Shabadin et al., 2014). Eq(8) represents the annual H_2 demand of the district which is estimated to be 1,141 kg.

$$\text{Annual } H_2 \text{ demand} = \frac{\text{Annual kilometres travelled} \times \text{No. of } H_2 \text{ vehicles} \times \text{Vehicle fuel economy}}{H_2 \text{ gravimetric energy density}} \tag{8}$$

3.1 Results and Discussion

The optimised network design has an annual system cost of approximately USD 16.3 million with energy consumption of 10 MW. The H_2 production plant requires 293 t of palm oil mill effluent and 16 t of water to achieve the desired production rate. Referring to the H_2 supply chain cost breakdown in Figure 3, H_2 purification technologies represent the highest percentage of the total system cost.

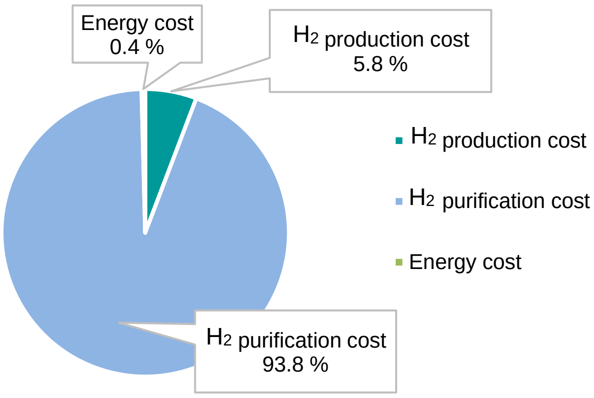

Figure 3: Cost breakdown of the optimised supply chain configuration

Technical standards SAE J-2719 (2020) and ISO 14687 (2019) mandate that the minimum H_2 purity required for automobile applications is 99.99 %. Cryogenic air separation units are required to purify H_2 (Kotchourko and Jordan, 2022). This corroborates with the trend shown in the energy consumption breakdown in Figure 4, whereby H_2 purification has the highest energy consumption.

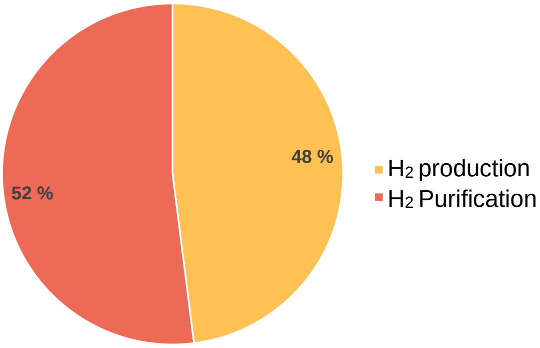

Figure 4: Energy breakdown of the optimised supply chain configuration

The optimisation result selected cryogenic separation instead of other H_2 purification methods, such as membrane technologies, because the polymeric membranes utilised in membrane separation technologies display high energy efficiency but have an overall lower separation efficiency than cryogenic separation due to the limitations in H_2 permeability and H_2/biomethane selectivity (Lu et al., 2020). More membrane modules will be required for a multistage purification system to achieve the equivalent purity requirements for the H_2 product, increasing total equipment costs.

It should be noted that the temporal availability of biomass feedstock will influence the optimal H_2 production method chosen by the mathematical model. The biomass characteristics also affect the production efficiency and final H_2 yield. As more byproducts are generated due to the impurities present in the feed, additional pretreatment and downstream purification units may be required, which may subsequently affect the overall cost and energy consumption of the H_2 plant.

4. Conclusions

The mathematical model presented generated an optimised green H_2 supply chain with a liquid NH_3 synthesis loop for H_2 storage and distribution for maximum economic performance. The simulation results indicate that the dark fermentation of POME is the most cost-effective hydrogen production pathway, and the optimised network design has a system cost of approximately USD 16.3 million and an energy consumption of 10 MW. In order to meet the transportation requirement, membrane technology is selected to purify H_2 to 99.99 %. Given the techno-economic results attained, NH_3 is a feasible option as an energy carrier for green H_2 supply chains at a national level. Future feasibility studies and preliminary planning of national H_2/NH_3 energy systems may incorporate two-layer or multi-objective optimisation models to address the inherent compromises between potentially conflicting objectives.

Nomenclature

CAPEX_b – capital cost of technology *b*, USD
CAPEX_d – capital cost of technology *d*, USD
Cost_b – total associated costs of technology *b*, USD/y
Cost_d – total associated costs of technology *d*, USD/y
e_{abc} – energy consumption factor of technology *b*, kWh
e_{cde} – energy consumption factor of technology *d*, kWh
EN_b – energy consumption of technology *b*, kWh
EN_d – energy consumption of technology *d*, kWh
F_{ac} – mass flow rate of feed *a*, kg/h
F_c – mass flow rate of intermediate product *c*, kg/h
F_e – mass flow rate of product *e*, kg/h
OPEX_b – operating cost of technology *b*, USD/h
OPEX_d – operating cost of technology *d*, USD/h
x_{abc} – component mass conversion of the inlet feed *a* of technology *b* to intermediate product *c*,
x_{cde} – component mass conversion of the inlet feed *c* of technology *d* to the final product *e*, -
z_b – number of units of technology *b* selected, -
z_d – number of units of technology *d* selected, -

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References

Andersson J., Grönkvist S., 2019, Large-scale storage of hydrogen, International Journal of Hydrogen Energy, 44(23), 11901–11919.

Brun K., Allison T.C. (Eds), 2022, Machinery and Energy Systems for the Hydrogen Economy, Elsevier, Amsterdam, Netherlands, ISBN: 9780323903943.

ISO Technical Committee, 2019, ISO 14687:2019 Hydrogen fuel quality — product specification, ISO Technical Committee, United States. <www.iso.org/standard/69539.html>, accessed 04.07.2023.

Kotchourko A., Jordan T. (Eds), 2022, Hydrogen Safety for Energy Applications: Engineering Design, Risk Assessment, and Codes and Standards, Butterworth-Heinemann, Oxford, UK., ISBN: 9780128204924.

Kojima Y., 2019, Hydrogen storage materials for hydrogen and energy carriers. International Journal of Hydrogen Energy, 44, 18179–18192.

Lim H.P., 2019, S'wak launches first integrated hydrogen production plant, refuelling station in Southeast Asia, <www.theborneopost.com/2019/05/27/swak-launches-first-integrated-hydrogen-production-plant-refueling-station-in-southeast-asia/>, accessed 28.07.2022.

Lu H.T., Wen L., Miandoab E.S., Kanehashi S., Hu G.P., 2020, The opportunity of membrane technology for hydrogen purification in the Power to Hydrogen (P2H) roadmap: A review. Frontiers of Chemical Science and Engineering, 15(3), 464–482.

Mah A.X.Y., Ho W.S., Phun C.B., Hassim M.H., Liew P.Y., Asli U.A., Kamaruddin M.J., Chemmangattuvalappil, N.G., 2019, Review of hydrogen economy in Malaysia and its way forward. International Journal of Hydrogen Energy, 44(12), 5661–5675.

Mah A.X.Y., Ho W.S., Hassim M.H., Hashim H., Liew P.Y., Asli U.A., Muis Z.A., Hoh G.T.L., 2020, Optimization of hydrogen supply chain: A case study in Malaysia. Chemical Engineering Transactions, 78, 85-90.

Makepeace J.W., He T., Weidenthaler C., Jensen T.R., Chang F., Vegge T., David W.I.F., 2019, Reversible ammonia-based and liquid organic hydrogen carriers for high-density hydrogen storage: recent progress, International Journal of Hydrogen Energy, 44(12), 7746–7767.

Mori D., Hirose K., 2009, Recent challenges of hydrogen storage technologies for fuel cell vehicles, International Journal of Hydrogen Energy, 34(10), 4569–4574.

Palma V., Barba D., Vaiano V., Colozzi M., Palo E., Barbato L., Cortese S., Miccio M., 2018, Catalytic Oxidative Decomposition of H_2S for Hydrogen Production, Chemical Engineering Transactions, 70, 325-330.

SAE Standards, 2020, Hydrogen fuel quality for fuel cell vehicles. SAE International, United States, <www.sae.org/standards/content/j2719_202003/>, accessed 03.07.2023.

Shabadin A., Megat N., Jamil H.M., 2014, Car annual vehicle kilometer travelled estimated from car manufacturer data – an improved method, Pertanika Journal of Science & Technology, 25(1), 171-180, <myjurnal.mohe.gov.my/filebank/published_article/57395/13.pdf>, accessed 03.07.2023.

Suruhanjaya Tenaga, 2019, National Energy Balance 2019, Suruhanjaya Tenaga, Malaysia. <meih.st.gov.my/documents/10620/19759/National+Energy+Balance+2019>, accessed 03.07.2023.

Toyota Europe Newsroom, 2021, Toyota Mirai breaks world record for distance driven with one fill of hydrogen, <newsroom.toyota.eu/toyota-mirai-breaks-world-record-for-distance-driven-with-one-fill-of-hydrogen/>, accessed 21.03.2023.

Valera-Medina A., Xiao H., Owen-Jones M., David W.I.F., Bowen P.J., 2018, Ammonia for power. Progress in Energy and Combustion Science, 69, 63–102.

Wong J., 2022, Sarawak gets into hydrogen-powered fuel cell electric vehicles. <thestar.com.my/business/business-news/2022/08/01/sarawak-gets-into-hydrogen-powered-fuel-cell-electric-vehicles>, accessed 27.03.2023.