TECHNICAL AND ECONOMIC OPTIMISATION OF THE RENEWABLE HYDROGEN PRODUCTION CHAIN FOR USE IN AMMONIA PRODUCTION IN MINAS GERAIS

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ABSTRACT

This work aims to assess the economic viability of the proposed renewable hydrogen production systems for use in ammonia production in Minas Gerais. Using mixed integer linear programming with LINGO 20® and Excel® software, the optimisation model confirmed the viability of the ammonia production routes, demonstrating the profitability of the project. The highest investment was identified in case 3 (406 \$/tonne.NH_3), offset by the low cost of the raw material. Cases 2 and 4 had lower investments. Case 4 stood out for its shorter payback time (1 year) and lower production cost (445.7 \$/ton.NH_3), due to low logistical and operational costs, while cases 3 and 1 had production costs of 566.23 and 1414.45 \$/ton.NH_3, respectively, with payback times of 5 years, both within the maximum limit of 5 years considered attractive. Long-term economic sustainability depends on continuous optimisation and the management of costs specific to each project.

Keywords: Biomass gasification, Steam reforming, Water electrolysis, Resource transportation, Optimization.

INTRODUCTION

The production of green ammonia uses renewable energy sources to obtain clean hydrogen, which is combined with atmospheric nitrogen. Technologies such as water electrolysis, anaerobic digestion and biomass gasification have been used to generate low-carbon energy and fuels, reducing greenhouse gas emissions. After implementing these technologies, adjustments are needed to increase accuracy and efficiency. Modelling and optimisation are key tools for improving decision-making in areas such as engineering and logistics. This work aims to assess the economic viability of the proposed renewable hydrogen production systems for use in ammonia production in Minas Gerais.

MATERIALS AND METHODS

The methodology was based on mixed integer linear programming, governed by the objective function (Equation 1), implemented in LINGO 20®

software, with Excel® as the interface for data input and output.

$$MIN = ann.Inv + RMC + TC - P.Rev \qquad Eq.\ (1)$$

ann. Inv – Annualised investment, RMC – raw material costs, TC – Transport cost and P.Rev – Production revenue

To solve the objective function, mass balance restrictions were applied, ensuring that the inflows and outflows are equivalent, in accordance with the law of conservation of mass. Availability and demand constraints ensured access to resources in each region and complete fulfilment of demand. Transport restrictions were also added, considering the use of lorries to manage material flows. Financial calculations included net present value (NPV), Equation 3, discounted cash flow (Equation 2), internal rate of return (IRR), Equation 4 and discounted payback (Equation 5), using specific equations for each indicator.

$$Discounted\ cash\ flow\ in\ year\ time = \frac{Cash\ flow}{(1+Discount\ rate)^{time}} \qquad \text{Eq. (2)}$$

$$VPL = \sum Discounted\ cash\ flow\ in\ year\ time - Initial\ investment \qquad \text{Eq. (3)}$$

$$0 = \sum \frac{Cash\ flow_{time}}{(1+TIR)^{time}} - total\ investment \qquad \text{Eq. (4)}$$

$$Initial\ investment - \sum Discounted\ cash\ flow\ in\ year\ time \geq 0 \qquad \text{Eq. (5)}$$

The calculation of the total investment was based on the authors' cost references [1], [2], [3]; [4] e [5]. The plant was adjusted to an optimised scale with a factor of 0.6, reflecting economies of scale, where increasing the size reduces the investment per unit of production. The cost of transporting the woody biomass was calculated using a lorry with a capacity of 40m^3 [6], The hydrogen consumption was calculated on the basis of a lorry with a capacity of 39.6m^3 at 200 bar [7], of ethanol and vinasse was based on a truck with a capacity of 50,000 litres [8]and biomethane based on a 5.8 tonne lorry [9] capacity, considering a distance of 100 km and an average diesel consumption of 3 litres/km [10]. With these parameters, we arrived at a cost of 32.9 $/tonne.100km for woody biomass, 480.7 $/tonne.100km for transporting hydrogen gas, 6.7 $/tonne.100km for transporting ethanol and 5.3 $/tonne.100km for transporting vinasse.

Physical, economic and logistical models were developed to optimise the main hydrogen production routes for ammonia production. This required the use of an air separation unit (ASU) to obtain nitrogen, as well as a unit for ammonia synthesis (HB). The physical model is represented by the input and output mass flows to optimise hydrogen production for ammonia production, without detailing intermediate processes due to the format of the optimisation model developed, which focuses exclusively on these variables. The economic model is related to data on the purchase and sale of raw materials (water, electricity, hydrogen, ammonia, woody biomass and ethanol), as well as transport and investment costs, with the aim of minimising costs throughout the project, and the logistics model, which optimises distribution routes, taking into account the demand and availability of resources, determining the best locations for production, transport of resources to make intermediate conversions and sale of the final product, with the aim of efficiency and reducing logistics costs. To analyse the data, cases were developed, namely: case 1- Electrolyser PEM(PEM+HB) [1] ; case 2 - Gasification of wood waste (GS_SMR+HB) [2]; caso 3- Vinasse digestion and biomethane SMR (Vinasse_BD_SMR+HB) [3] [4]; case 4 - ethanol SMR (Ethanol+SER+HB) [5]. The study was carried out in the state of MG, in the 66 micro-regions, where the demand for ammonia was established, based on Brazil's annual production which corresponds to 1,500,000 tonnes/year, with a restriction in the code to ensure that total production does not exceed this capacity. The analysis in this work covers a period of 20 years, with an interest rate of 12% p.a. based on the minimum Selic rate. Although the price of grey ammonia varies between 900 and 1,200 $/ton [11], in this study, a higher value of $1,500/tonne was assumed for renewable ammonia.

RESULTS AND DISCUSSION

Figure 1 compares the investment, raw material cost, transport cost and sales revenue for different ammonia production technologies. Each technology uses a specific raw material and process to produce the hydrogen that will be used in ammonia production.

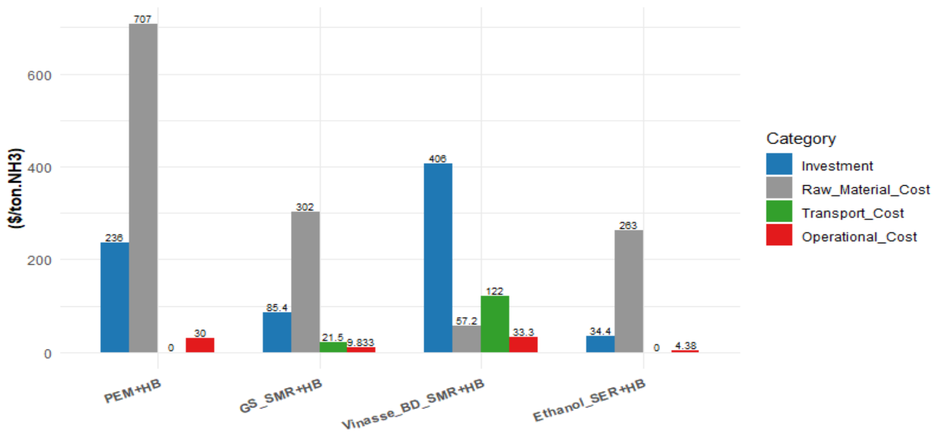

Fig. 1. Comparative analysis of ammonia production technologies.

The optimisation model, based on the established conditions, identified all the ammonia production routes as viable, demonstrating the profitability of the project from the outset. In case 3, the Paracatu and Uberaba micro-regions were chosen for ammonia production, making use of vinasse, an abundant by-product of the ethanol industry, which reduces the cost of the raw material. However, the high investment required (3983.62 M$) for the infrastructure to convert vinasse into biomethane reduces the attractiveness of the technology. The transport of biomethane and vinasse generated the second highest cost, at 122 $/ton.$NH_3$. With a payback of 5 years and an IRR of 17%, the financial return is slower, but the use of agro-industrial waste offers environmental and sustainability advantages. Similarly, case 1, which has a slower payback time of 5 years and an IRR of 18%, provides a higher return on investment. Case 1 has the second highest investment at 3584.97 M$ due to the use of PEM electrolysis cells. The high raw material cost (707 $/ton.$NH_3$) is attributed to the high electricity consumption for electrolysis, coupled with high operating costs. An ammonia production plant was designed to be installed in Juiz de Fora, which eliminates logistical costs as it is strategically located in a region with easy access to raw materials to meet demand. Case 4 is the most advantageous, with the lowest investment of $523.46 million, due to the availability of ethanol for hydrogen production and the use of mature technologies for its reforming. This results in low operating costs (4.38 $/ton.$NH_3$) and no logistical costs, thanks to the plant's strategic location (Ituiutaba and Uberaba). Although the cost of the raw material is 283 $/ton.$NH_3$, mainly due to the purchase of ethanol and electricity, the extremely high IRR of 305% and the 1-year payback make this technology highly profitable, especially in regions with an abundance of ethanol, such as Brazil. In case 2, the micro-regions of Salinas, Capelinha, Uberlândia, Três Marias, Conceição do Mato Dentro, Paracatu and Caratinga were chosen for ammonia production, with an investment of 2,843.74 M$. The highest cost is related to the raw material (302 $/ton NH3) due to the purchase of woody biomass, which also impacts the transport cost (9.8 $/ton.$NH_3$) to move hydrogen and biomass to the plant. With a payback of 3 years and an IRR of 33%, the project offers good profitability. The use of forest biomass is advantageous because it is renewable, but it is necessary to assess the environmental impact of wood degradation to ensure long-term sustainability. Although cases 1 and 3 shows a longer payback, both are within the attractive 5-year limit, which still makes them viable from an economic point of view. In terms of Net Present Value (NPV), case 4 is the most profitable, due to the low initial investment, which reduces the impact of fixed costs over time. Case 2 follows, with lower investment, an IRR higher than the mandatory discount rate and a relatively short payback period. Cases 1 and 3, on the other hand, have the lowest NPVs, due to the high initial investment and high raw material costs, which prolong the payback and reduce the financial competitiveness of these technologies.

Table 1. Financial analysis of production technologies.

Production technology	Total investment(M$)	NPV(M$)	Discouted payback(Years)
PEM+HB	3,584.97	649.04	5
GS_SMR+HB	2,843.74	997.39	3
Vinasse_BD_SMR+HB	3,983.62	696.26	5
Ethanol_SER+HB	523.46	1,651.18	1

In terms of production cost, case 1 has the highest value, at 1414.47 $/ton *$NH_3$*, partially above the cost of producing ammonia from grey hydrogen, which varies between 361.00 and 1300.00 $/ton [12]. Although higher, this is offset by the fact that it is a renewable technology with lower greenhouse gas emissions, making it competitive. Cases 2, 3 and 4 have costs of 1000.19 $/ton, 566.23 $/ton and 445.7 $/ton, respectively, all within the range of grey ammonia, with case 4 being the most competitive.

CONCLUSION

Case 4 shows the most promise in all the analyses made, with the shortest payback time. On the other hand, cases 1 and 3 may require interventions and subsidies to reduce their operating costs and payback. Based on the results of the financial analysis of all the cases, the project shows significant attractiveness, with a positive NPV, a high IRR and a payback period within the maximum limit, considered attractive, suggesting that the project not only recovers the initial investment in a reasonable period, but also generates high profits throughout its life cycle. In short, long-term economic sustainability depends not only on the initial choice of technology, but also on the continuous optimisation and efficient management of operational and logistical costs, taking into account the specific context of each project, including availability of raw materials, geographical location, and possible subsidies.

REFERENCES

[1] M. Jain, R. Muthalathu, and X. Y. Wu, "Electrified ammonia production as a commodity and energy storage medium to connect the food, energy, and trade sectors," *iScience*, vol. 25, no. 8, Aug. 2022, doi: 10.1016/j.isci.2022.104724.

[2] Y. K. Salkuyeh, B. A. Saville, and H. L. MacLean, "Techno-economic analysis and life cycle assessment of hydrogen production from different biomass gasification processes," *Int J Hydrogen Energy*, vol. 43, no. 20, pp. 9514–9528, May 2018, doi: 10.1016/j.ijhydene.2018.04.024.

[3] J. E. I. CUAN, "OTIMIZAÇÃO DE BIORREFINARIAS INTEGRADAS DE CANA-DE-AÇÚCAR E MICROALGAS UTILIZANDO PROGRAMAÇÃO LINEAR INTEIRA MISTA," 2023.

[4] C. Song, Q. Liu, N. Ji, Y. Kansha, and A. Tsutsumi, "Optimization of steam methane reforming coupled with pressure swing adsorption hydrogen production process by heat integration," *Appl Energy*, vol. 154, pp. 392–401, Sep. 2015, doi: 10.1016/J.APENERGY.2015.05.038.

[5] P. Khamhaeng, N. Laosiripojana, S. Assabumrungrat, and P. Kim-Lohsoontorn, "Techno-economic analysis of hydrogen production from dehydrogenation and steam reforming of ethanol for carbon dioxide conversion to methanol," *Int J Hydrogen Energy*, vol. 46, no. 60, pp. 30891–30902, Sep. 2021, doi: 10.1016/J.IJHYDENE.2021.04.048.

[6] D. P. Garcia, J. C. Caraschi, and G. Ventorim, "CARACTERIZAÇÃO ENERGÉTICA DE PELLETS DE MADEIRA," May 2013.

[7] J. D. Hunt and B. Salgado, "Aspectos sobre o armazenamento e transporte de hidrogênio," 2023. [Online]. Available: https://www.researchgate.net/publication/378078577

[8] Gestran, "O que é caminhão tanque e como é sua legislação?" Accessed: Sep. 29, 2024. [Online]. Available: https://www.gestran.com.br/blog/o-que-e-caminhao-tanque-e-como-e-sua-legislacao

[9] Gasprom, "Carreta de GNC 2024: Máxima Capacidade e Eficiência!" Accessed: Oct. 14, 2024. [Online]. Available: https://gasprom.com.br/equipamentos-/carreta-de-gnc/

[10] É. Pimenta, "Quanto custa encher o tanque de um caminhão no Brasil?" Accessed: Sep. 16, 2024. [Online]. Available: https://autopapo.com.br/noticia/quanto-custa-encher-o-tanque-de-um-caminhao-brasil/

[11] Alibaba, "preço da amônia líquida opções para os melhores preços acessíveis." Accessed: Oct. 13, 2024. [Online]. Available: https://portuguese.alibaba.com/g/liquid-ammonia-price.html

[12] H. Hein, "Amônia verde já é tão competitiva quanto combustíveis fósseis." Accessed: Oct. 14, 2024. [Online]. Available: https://canalsolar.com.br/producao-de-amonia-verde-ja-e-tao-competitiva-quanto-de-combustiveis-fosseis/