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Comparative Performance Analysis of Green Hydrogen Purification via Pressure Swing Adsorption and Supersonic Separation

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Hydrogen purification is a critical step in ensuring fuel quality for industrial and energy applications, particularly in processes following water electrolysis. This study compares two purification technologies—Pressure Swing Adsorption (PSA) and Supersonic Separation (SS)—through steady-state simulations in Aspen Plus. The PSA model was developed using literature-based adsorption parameters, while the SS model is a reduced-order version derived from Aspen HYSYS simulations and implemented using an Excel-integrated Calculator block. The evaluation considered hydrogen purity, energy demand, operational feasibility, and scalability. PSA achieved 99.999% purity with 99.7% efficiency, whereas SS reached 99.95% efficiency under similar conditions. While PSA relies on dual-column cycling with adsorbent regeneration, SS uses high-speed expansion to induce phase change and simplify water removal. The absence of adsorbent use in SS reduces material costs and maintenance needs, though it demands precise thermodynamic control. The findings provide insights into selecting purification technologies based on energy efficiency, system complexity, and throughput, supporting decision-making in green hydrogen production chains.

* 1. Introduction

Green hydrogen, produced via electrolysis, is increasingly recognized as a key energy carrier in the transition to a low-carbon economy. In this process, electricity from renewable sources is used to split water molecules, producing hydrogen without emission of greenhouse gases. Despite its growing industrial use, the widespread adoption of green hydrogen still faces significant challenges, particularly due to the high costs associated with its production, storage, transportation, and the substantial electricity demand (Dos Santos et al., 2023).

Among these challenges, achieving the required hydrogen purity is crucial, as many industrial applications—particularly fuel cells—require exceptionally high-purity hydrogen. Hydrogen produced via electrolysis contains trace impurities such as oxygen (O₂) and water vapor (H₂O), which must be removed to meet the purity requirements established by ISO 14687:2019. Insufficient purification can significantly impact the efficiency of downstream processes. Therefore, the development of innovative and highly efficient purification technologies is essential (Santana et al., 2023).

To meet these purity requirements, integrated systems combining catalytic deoxidation (Deoxo) and Pressure Swing Adsorption (PSA) are commonly employed. PSA is a well-established technology that exploits the differential affinities of gases for adsorbent materials under varying pressures, providing high selectivity in impurity removal. However, limitations remain, including semi-continuous operation, frequent regeneration requirements, and efficiency losses due to pressurization and incomplete adsorption (Du et al., 2021; Zito et al., 2015).

To address some of these limitations, Supersonic Separators (SS) have been applied in natural gas purification and are emerging as a promising alternative for hydrogen purification. SS operates via adiabatic gas expansion in Laval nozzles, enabling selective condensation and centrifugal removal of impurities. This process is continuous, compact, and does not rely on adsorbents or regeneration cycles, with extremely short residence times (Cao & Bian, 2019; Ávila et al., 2022).

Despite the maturity adsorption and supersonic separation technologies, there is a lack of comparative studies in the literature evaluating these methods for hydrogen purification. Most studies focus on various applications of PSA in systems targeting hydrogen purity and process optimization, while SS has predominantly been applied to gas streams in oil and gas processing. Therefore, cost estimation remains highly uncertain when comparing both technologies, and the impact of SS modifications on the levelized cost of hydrogen has been scarcely investigated (Burguers et al. 2022; Shooshtari & Shahsavand, 2023).

This study presents a comparative analysis of the performance of two purification methods—Pressure Swing Adsorption (PSA) and Supersonic Separation (SS)—with a focus on their technical efficiency and potential impact on the overall cost of hydrogen production. Both models were developed in Aspen Plus, supported by a custom Excel extension. The PSA model is based on literature data concerning hydrogen adsorption, whereas the SS model was implemented as a reduced-order model derived from Aspen HYSYS simulations. The analysis focuses on the purification stage following the deoxidizer unit in electrolyzer-based hydrogen production.

* 1. Methodology

This study is structured into three phases: (I) the PSA model, (II) the SS model, and (III) the performance criteria. Each of these steps will be explored in detail in the following subsections, which outline the modeling techniques and parameters used to evaluate the efficiency of the hydrogen purification processes.

In addition to the steps discussed in the subsequent sections, the Proton Exchange Membrane (PEM) electrolyzer model was developed as a plug-in in Aspen Plus v.14 to provide the input for the PSA and SS models (Bispo et al., 2024). The hydrogen production stream from the PEM electrolyzer serves as the input stream for both the PSA and SS purification processes, ensuring an integrated approach to the study.

The base plant capacity is 200 MW, aligned with the operational scales of real-world projects currently under development in Brazil, as outlined in recent reports by the National Confederation of Industry (CNI, 2024). This scale is consistent with large-scale, industrial hydrogen production systems and provides a practical basis for the analysis of hydrogen purification methods in real-world applications.

* + 1. PSA model

Although the PSA process is inherently transient, it was represented in Aspen Plus® using a steady-state approximation through a customized model. This model adopts a hierarchical structure incorporating a Calculator routine, which estimates H₂ and water outputs based on the degree of H₂ purification, operating pressure, and temperature, and the characteristics of the NaX adsorbent (Zito et al., 2015). NaX refers to the three-letters identification code adopted by the International Zeolite Association and identifies different structures and properties of the adsorbent material.

The adsorption behavior of H₂ and water on NaX was derived from experimental isotherms and modeled using multivariate regression fitted to the Langmuir equation. Within the Calculator block, the model uses adsorbent properties and the inlet stream conditions (temperature, pressure, and composition) to predict the performance of the PSA unit.

Assuming a fixed amount of 1 ton of adsorbent per column, the model determines the number of columns required, the amount of retained components, and the flow rate of the purified hydrogen stream.

* + 1. SS model

The SS model was implemented in Aspen Plus® as a reduced-order model, built from simulations carried out using an in-house Unit Operation Extension (UOE) developed in Aspen HYSYS®. This UOE was designed to represent the full thermodynamic behavior of the SS, simulating the process from the adiabatic expansion of the gas stream to the subsequent subsonic recompression, enabling the prediction of condensed phase formation and its separation from the gas phase. The model was developed as part of a research project at SENAI CIMATEC University.

The UOE receives as input variables the temperature, pressure, and composition of the feed stream, along with several SS specification parameters such as the shock Mach number, internal diameters, and lengths of the converging and diverging sections of the SS. As output, the UOE provides the temperature, pressure, and composition of the separated streams, as well as other relevant design variables, including the angles of the converging and diverging sections, the inlet Mach number, the throat area of the SS, and the shock temperature and pressure.

Based on the results generated by the UOE, a multivariate regression was performed to construct a simplified predictive model, which was then integrated into Aspen Plus® via a Calculator block. This reduced-order model allows efficient estimation of SS performance under varying operating conditions while preserving the thermodynamic behavior captured in the original simulations.

In Aspen Plus®, the model returns the composition, temperature, and pressure of the purified hydrogen stream, along with the estimated values of recovery and separation efficiency based on the specified operating conditions.

* + 1. Performance criteria

Performance criteria are evaluated based on hydrogen purity and levelized cost. Initially, both PSA and SS strategies are designed to meet the 200 MW plant specifications, and their performance outcomes are quantified; a sensitivity analysis is performed varying hydrogen production for 100 MW and 300 MW. Subsequently, each strategy's key equipment, raw materials, and utilities costs are also considered. Finally, the implementation of SS is assessed as a potential modification to the conventional electrolysis process by accounting for the impact on the levelized hydrogen purification cost if SS is implemented.

The supersonic separator equipment cost is estimated according to Equation (1) (Magalhães 2019). Since the input of the SS model is dimensioned according to PEM electrolysis outlet quality and operational conditions, only CAPEX and an O&M of 10% CAPEX is assumed. O&M cost is related to the maintenance of the SS structure and general expenses; A 10% estimate is adopted as a reasonable assumption, given the limited number of studies available in the literature regarding the application of supersonic separation (SS) in electrolysis processes.

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| $$C\_{SS}(\$)=6,071,100\*\left(\frac{C\_{(m^{3}/h)}}{250,000}\right)^{0.6}\*\left(\frac{P\_{\left(bar\right)}}{80}\right)^{0.6}$$ | (1) |

Pressure Swing adsorption process mainly requires electrical energy for operation and sorbent material. Therefore, the CAPEX and OPEX of the PSA system were estimated based on a regression analysis of data reported by the Bay Area Air Quality Management District (2025) and LCRI (2024). The annual OPEX was assumed to correspond to 0.0105 $/kg H2, accounting for sorbent replacement and pressure vessel operational costs. Figure 1 presents the linear equation obtained.



Figure 1: CAPEX PSA unity (US$) x PEM electrolysis Size (MW)

For the levelized cost of purification (LCOP), as given by Equation (2), only the purification section is considered, including its auxiliary components from process simulation. The hydrogen flow, expressed in kilograms per hour, is calculated for one year of operation, assuming 8,000 hours, and a 20-year plant lifetime.

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| $$LCOP= \frac{C\_{CAPEX}+C\_{OPEX}}{\dot{m}\_{H\_{2}}h}$$ | (2) |

* 1. Results and discussion

This section presents the purity levels achieved by each purification technology evaluated in the study. The results include the residual concentration of water in the purified hydrogen stream, as well as the amount of hydrogen retained or lost in the captured impurity stream. Figure 2 summarizes the two alternative hydrogen purification technologies, providing a comparative overview of their operational configurations and performance. The corresponding quantitative data are organized and detailed in Table 1, allowing for a clear assessment of each technology’s effectiveness in achieving the desired hydrogen purity specifications.



Figure 2: Overall Process Flow.

Table 1: PSA and SS stream composition

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|   | **H2 stream purified flow** | **H2 stream captured flow** |
|  | SS (%f mass) | PSA (%f mass) | SS (%f mass) | PSA (%f mass) |
| 100 MW | >0,99999 | >0,99999 | 0,1030 | 0,0979 |
| 200 MW | >0,99999 | >0,99999 | 0,0185 | 0,0979 |
| 300 MW | >0,99999 | >0,99999 | 0,0252 | 0,7600 |
|   | **PEM mass outlet x stream captured flow loss of H2 in mass** |
|  | PEM outlet (%f mass) | PEM (kg/h) | SS (kg/h) | PSA (kg/h) |
| 100 MW | 0,99950 | 1840,29 | 0,11 | 0,21 |
| 200 MW | 0,99950 | 3680,58 | 0,04 | 0,21 |
| 300 MW | 0,99950 | 5520,87 | 0,06 | 0,21 |

It is possible to observe in *Table 1* - *H2 stream purified flow* that for automotive applications, which have a purification requirement of 5S (99,999%) after the decimal point, both technologies achieve their objective at all scales. In *Table 1* - *H2 stream captured flow*, in the capture stream, it is possible to identify that for the scales studied, the SS has a smaller amount of H2 loss, with the exception of the 100 MW scale, which can be associated with a lower total flow rate of the system for capacities of 100 MW, which can result in a higher H2 concentration in the capture stream. Finally, in *Table 1* - *PEM mass outlet x stream captured flow loss of H2 in mass*, the analysis is verified in terms of the mass of H2 produced in the PEM x mass of H2 lost in each purification system, in which a lower loss in general is observed in the SS and a constancy of values in the PSA, which operated with two final columns. After the technical analysis, economic performance criteria are evaluated. CAPEX and LCOP for each strategy are presented in *Table 2*.

*Table 2: PSA and SS Economic comparison.*

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|   | **PSA and SS CAPEX** | **LCOP comparison for PSA and SS strategy** |
|  | SS CAPEX | PSA CAPEX | SS (US$/kg) | PSA (US$/kg) |
| 100 MW | US$115,333.02 | US$5,007,545.41 | 0.0012 | 0.0275 |
| 200 MW | US$174,812.17 | US$8,182,849.58 | 0.0009 | 0.0488 |
| 300 MW | US$222,959.72 | US$11,358,153.76 | 0.0008 | 0.0701 |

The PSA system exhibited a significantly higher CAPEX compared to the SS strategy as presented at *Table 2 PSA and SS CAPEX*. However, the SS process primarily relies on electrical energy consumption, particularly due to the need for compression at the equipment inlet for product separation. In this study, the SS unit was designed based on the outlet conditions of PEM electrolysis, which results in no need of utility under normal operating conditions. These results suggest that proper integration and process design can yield a competitive total cost when compared to conventional PSA systems. Nevertheless, variations in process conditions may compromise the performance of the SS strategy, potentially resulting in reduced separation efficiency and suboptimal hydrogen purity, directly increasing the hydrogen purification final cost.

The comparison of the Levelized Cost of Hydrogen Production (LCOP) for Pressure Swing Adsorption and Supersonic Separation technologies reveals significant differences in cost at *Table 2* - *LCOP comparison for PSA and SS strategy*. For smaller capacities considered in this study (100 MW), the LCOP for PSA is 0.0275 US$/kg, while SS has a much lower LCOP of 0.0012 US$/kg. As capacity increases to 200 MW and 300 MW, PSA's LCOP rises to 0.0488 and 0.0701 US$/kg, respectively, indicating diminishing returns with larger scale. In contrast, SS maintains a low LCOP, decreasing further to 0.0009 US$/kg at 200 MW and 0.0008 US$/kg at 300 MW. This shows that SS benefits from significant economies of scale, offering superior cost efficiency in larger-scale hydrogen production.

The results suggest that PSA becomes less cost-effective as plant size increases. In contrast, SS proves to be a more efficient purification method for large-scale hydrogen production, with a decreasing LCOP as capacity grows. These preliminary results suggest that supersonic separators have the potential to achieve significant cost reductions in hydrogen purification across various scales. However, the SS strategy still requires validation of its efficiency under varying inlet process conditions while maintaining the same equipment design, and therefore, a very low cost of process purification. Despite the cost differences, PSA remains a low-cost alternative among conventional purification methods, and its high Technology Readiness Level (TRL) in commercial applications establishes it as a mature and reliable option for electrolysis systems.

* 1. Conclusions

This study presented a comparative performance analysis between Pressure Swing Adsorption (PSA) and Supersonic Separation (SS) for the purification of green hydrogen produced via PEM electrolysis. Both technologies were evaluated in terms of hydrogen purity, hydrogen loss, capital expenditure (CAPEX), and the Levelized Cost of Purification (LCOP), across plant scales of 100 MW, 200 MW, and 300 MW. The results demonstrate that both PSA and SS achieved the required hydrogen purity level (>99.999%) as defined by ISO 14687:2019. However, SS exhibited superior performance in terms of hydrogen recovery, with mass losses as low as 0.04 kg/h at 200 MW, compared to a constant loss of 0.21 kg/h in PSA systems across all scales. CAPEX analysis revealed a significant cost difference, with SS units costing between US$ 115,333.02 and US$ 222,959.72, while PSA units ranged from US$ 5.0 million to US$ 11.4 million for the same capacities. Most notably, SS demonstrated a substantially lower LCOP: 0.0008–0.0012 US$/kg H₂ compared to PSA’s 0.0275–0.0701 US$/kg H₂. This trend indicates that SS offers greater economic scalability and cost efficiency in hydrogen purification for large-scale applications.

The significance of the presented work lies in offering the first detailed quantitative comparison between PSA and SS technologies applied specifically to post-electrolysis green hydrogen purification. By integrating reduced-order modeling, techno-economic analysis, and simulation-based validation, the study provides critical insights into the cost-performance trade-offs of each strategy. These findings support informed decision-making for the design of future hydrogen production plants and open avenues for the development of intensified purification processes using novel technologies such as SS.

Therefore, while PSA remains a mature and reliable technology, particularly in commercial environments, SS appears as a promising and cost-effective alternative for large-scale hydrogen purification. Continued development and validation of SS under dynamic inlet conditions will be crucial to confirm its robustness and industrial applicability.

* 1. Future Works
* Energy Integration of the Process (Pinch Analysis)

Future research should explore the integration of hydrogen purification technologies within the overall process energy system using pinch analysis. This approach can identify heat recovery opportunities, minimize energy consumption, and enhance overall process efficiency by optimizing heat exchanger networks and reducing utility requirements.

* Supersonic Separation for Combined O₂ and Water Removal

An important avenue for further study involves extending the supersonic separation (SS) method to simultaneously separate oxygen and water, potentially eliminating the need for the catalytic deoxidizer reactor stage. Investigating the feasibility of removing oxygen along with water in the SS unit could simplify the process flow, reduce capital and operational costs, and improve process intensification.

* Development of a More Robust PSA Model (Transient Modeling)

The current PSA model is based on steady-state assumptions. Future work should focus on developing a transient, dynamic PSA model that captures the time-dependent behavior of adsorption/desorption cycles, column switching, and pressure fluctuations. Such a model would allow for more accurate performance prediction, optimization of cycle times, and better control strategy development.

* + 1. Additional Suggestions

In addition to the primary analyses, it is recommended to assess long-term operational stability and the degradation effects of adsorbents on PSA performance. This would support a more accurate lifecycle cost analysis. Moreover, exploring hybrid purification systems that combine PSA and SS technologies could potentially maximize the benefits of both approaches, providing a more efficient purification solution. The investigation of advanced control and automation strategies is also essential to improve the flexibility and reliability of purification units, especially in varying production conditions. Lastly, examining the scalability of SS technology in industrial settings, with pilot-scale demonstrations and integration with renewable hydrogen sources, such as those derived from organic materials, would contribute to a deeper understanding of its industrial application potential.

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