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A techno-economic analysis framework for intensified modular systems

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Abstract
In this work, a novel systematic techno-economic analysis framework is proposed for costing intensified modular systems. Conventional costing techniques are extended to allow estimation of capital and operating costs of modular units. Economy of learning concepts are included to consider the effect of experience curves on purchase costs. Profitability measures are scaled with respect to production of a chemical of interest for comparison with plants of traditional scale. In the developed framework, a base case scenario is analyzed to identify the relevance of the economy of learning and cost parameters that are yet to be established for modular projects that will be deployed. Then, a sensitivity analysis step is conducted to define changes in relevant variables that benefit the construction of modular systems. In a final step, scenarios in which the modular technology presents break-even and further reduction in cost are identified. A process model for a modular hydrogen unit is developed and used for demonstration of the proposed framework. In this application, process synthesis is carried out, including operability analysis for selection of feasible operating conditions. A comparison with a benchmark conventional steam methane reforming plant shows that the modular hydrogen unit can benefit from the economy of learning. A synthesized flowsheet for a modular steam methane reforming plant is used to map the decrease in natural gas price that must be needed for the plant to break even when compared to traditional technologies. Scenarios in which the natural gas price is low allow break-even cost for both individual hydrogen units and the assembled modular plant. For such break-even cases, the economy of learning must produce a reduction of 40% or less in capital cost when the natural gas price is under 0.02 US$/Sm^3. This result suggests that the synthesized modular hydrogen process has potential to be economically feasible under these conditions. The developed tools can thus be used to accelerate the deployment and manufacturing of standardized modular energy systems.

KEYWORDS
modular systems, process intensification, techno-economic analysis

1 | INTRODUCTION

Advances in process systems engineering, materials, catalysis, and reaction engineering have allowed the conceptualization of novel modular and intensified processes.[1–4] As a result, new emerging technologies enable promising capabilities, including more efficient and sustainable utilization of natural resources for production of value-added chemicals and energy. In particular, transportable and physically small modular systems consist of a potential solution to monetize resources available in challenging conditions; for example, short-term shale gas wells, stranded natural gas (NG), and resources that are abundant in remote geographic locations.

Process intensification can be interpreted as a comprehensive set of strategies to reduce the size of chemical processes, producing efficient designs in terms of conversion, utilities and energy consumption, as well as reduction of emissions, and waste disposal. The concepts of modularization in turn are usually limited to spatial configuration and the ability to manufacture a plant in the form of standardized modules for skid-mounted assembly and easy transportation. Recent studies have focused on the development of intensified modular designs for the conception of flexible yet efficient small modular plants.[4–6]

The deployment of commercial modular technologies presents a variety of challenges such as assuring feasible and profitable operations. Process modularization is often achieved with high degrees of customization. For such technologies, the application of conventional techno-economic analysis (TEA) methods is hindered because modular units present extremely low processing capacities in comparison with typical large-scale plants. These units also present integrated process topologies that differ from the one operation per unit scheme typically employed for costing of large-scale plants.[4]

Process integration and intensification may generate multifunctional modular units that stand out from their conventional counterparts in terms of efficiency and footprint. Moreover, drastic changes to heat integration and reaction rate improvements are likely to affect utilities generation and management. Consequently, comparative economic evaluation of highly integrated modular plants may only be possible in a plantwide manner, for example, by scaling total costs with respect to a certain chemical product for direct comparison to traditional plants.

Additional cost challenges derive from the concept of economy of scale. Traditional large-scale plant designs rely on the economy of scale, in which larger production capacities decrease the relative cost of production. Modular systems are disadvantaged by economies of scale because more construction material is required for smaller production volumes proportionally.

However, modular units are expected to be standardized and mass produced, unlike conventional-scale plants. As more modular units are manufactured, unit costs may decrease due to improvement in both individual manufacturing skills and organizational routines. First-of-a-kind designs are expected to have higher costs, whereas n^{th}-of-a-kind designs are presumably cheaper due to accrued know-how (or learning-by-doing) and manufacturing experience. Technological maturity is achieved when the costs to manufacture considered pieces of equipment steadily approach constant values. Notably, these reductions in cost are not spontaneous and must be managed.[7] In addition, with the numbering up phenomena becoming more common with the necessity for modularization, there is a critical need for investors to look at solid financial predictors as an attempt to reduce uncertainty with respect to their assets.[8]

Historically, experience curve techniques have been applied to describe the effect of the economy of learning on the purchase cost of the diverse technologies, ranging from cars to chemical plants.[7,9,10] In the scope of manufacturing modular units in the Chemical Engineering field, the incorporation of the learning aspects have been sparsely studied.[11–13] Moreover, the inclusion of economy of learning in the TEA of modular systems that are also intensified is yet to be addressed.

The consideration of economy of learning in modular manufacturing has potential to support the economic evaluation of more realistic scenarios. Nevertheless, requirements associated to costing data and experience curve parameters may prevent fast and effective techno-economic and profitability analyses. Particularly, capital and operating costs are commonly obtained from undisclosed price quotations, which are only conceivable to plant designs closer to completion. The economy of learning widely varies and depends on diverse factors such as research investment, market trends, process specifications, and so forth.[7]

This Article addresses cost challenges of intensified modular plants. A novel systematic TEA framework for modular systems is proposed for cost estimation and profitability with respect to conventional technologies. Classic concepts of engineering economic analysis for chemical processes are extended to include estimation of capital and operating costs of intensified modular plants based on available literature process design data.[14]

In particular, the economy of learning concept is newly introduced to cost analysis of modular systems. In this concept, the experience curve accounts for changes in modular system's purchase cost according to the number of manufactured modules. Cost estimations are divided into two scenarios according to experience curve models: (i) the experience curve is modeled based on previous modular deployment data; and (ii) the experience curve parameters are varied to achieve distinct profitability targets. The examination of the two cases provides competitivity insights and determines the situations in which the candidate modular technology is promising for future deployment or further research.

An application to a modular and intensified hydrogen production unit is considered. Process synthesis is carried out around an intensified microchannel reactor for steam methane reforming (SMR), which consists of an integrated alternative to the conventional unit operations of pre-reforming, reforming furnace, and high-temperature shift reactors. Operability analysis is employed to study feasible process operating regions and determine the nominal modular operation.[5,15]

Then, TEA of the hydrogen production unit is performed in comparison with an adopted conventional steam methane reforming plant. Measures of scaled equivalent annual operating cost (EAOC) are used to assess how competitive modular units are, independently of size and production capacity. A supplementary investigation is also presented supposing bulk purchase of modular units to attain the same hydrogen production as the conventional plant.

The rest of this Article is structured as follows: In Section 2, the economy of learning model is introduced; in Section 3, the modular TEA framework is discussed; in Section 4, the modular hydrogen unit application is addressed; finally, in Section 5, conclusions are drawn, and future directions are presented.

2 | ECONOMY OF LEARNING CONCEPTS

Economies of learning rely on the concept of experience curves to account for the effects of the level of maturity on the cost of the manufactured technology. The economy of learning is also known as the economy of mass production and the economy of numbers because it considers the mass production behavior in manufacturing. Unit prices tend to decrease with expansion in cumulative production output due to continuous manufacturing improvements.[16]

The experience curve is a generalization of the learning curve concept. Learning curves are associated with reductions in cost of labor due to gained labor skills over worked hours. Experience curves consider overall cost savings due to improvement in various organizational routines including individual skills, manufacturing techniques, innovation, and so forth. While the learning curve is generally used to forecast labor costs, the experience curve is a strategic tool to manage cost reductions as units are manufactured.[7] Several shapes have been proposed for the experience curve that represent the economy of learning.[9] For example, the power law function has been used to represent the experience curve and the economy of learning. Here, the power law function is adapted to explicitly include a plateau effect as follows[10]:

$$F_n = 1 - R_n = \begin{cases} n^{-\alpha}, & \text{if } n^{-\alpha} \geq R_{max} \\ R_{max}, & \text{if } n^{-\alpha} < R_{max} \end{cases} \tag{1}$$

$$C_n = F_n \cdot C_1 \tag{2}$$

where F_n is a purchase cost factor that represents the reduction in purchase cost, R_n $(0 \leq R_n < 1)$ is the reduction in purchase cost, $n \in \mathbb{N}$ $(n \geq 1)$ is the number of manufactured units, α is an experience rate exponent, R_{max} is the maximum reduction in purchase cost, and C_n is the purchase cost of the nth manufactured unit. R_{max} corresponds to a plateau in the experience curve, in which the technology achieves maturity. Note that the purchase cost factor F_n is a multiplier that indicates no cost reduction for the first-of-a-kind unit, that is, $F_1 = 1$ or 100% of initial cost and $R_1 = 0$ or 0% reduction.

Figure 1 illustrates the experience curve for a situation in which a maximum reduction in cost of $R_{max} = 30\%$ and an experience rate exponent $\alpha = 0.15$ are assumed. In this example, the experience curve plateau and technology maturity happen around the 11th unit.

In this work, α, R_{max} and n are referred to as experience parameters. The values of α and R_{max} are initially fitted to literature values of F_n for evaluation of a base case scenario. Then, through further studies, the experience curve is shaped for competitiveness with respect to benchmark technologies.

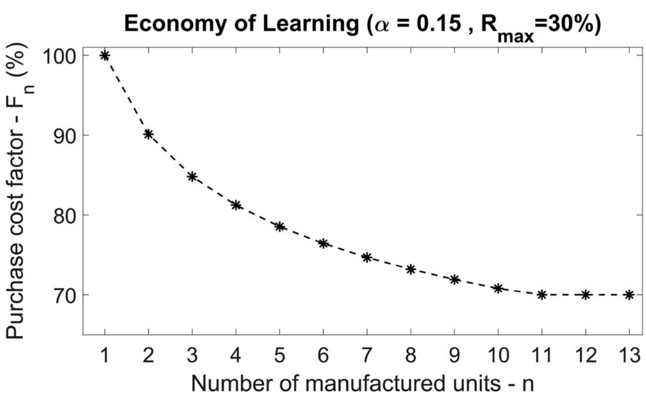

FIGURE 1 Illustration of the experience curve considering $\alpha = 0.15$ and $R_{max} = 30\%$

3 | PROPOSED MODULAR TEA FRAMEWORK

The proposed framework extends existing cost correlations to include intensified modular systems. At first, a compatible conventional technology is adopted as benchmark for cost comparison. Then, modular and conventional process flowsheet specifications are considered, and estimations of capital and operating costs of both technologies are performed. Adaptation of traditional costing methods are developed for the modular technology so that reference values associated with conventional plants can be employed along with the economy of learning concepts.

The cost estimation is divided into two scenarios: (i) a base case scenario, in which experience parameters are estimated using literature data; and (ii) profitability scenarios, in which experience parameters are varied together with other significant variables to achieve break-even and further cost reductions. The division into these scenarios is motivated by the fact that the experience curve should be managed as pointed out above. Therefore, the base case scenario is used for an initial cost performance analysis that determines if the economy of learning and other parameters should be considered for profitability. In case the unit price reduction due to economy of learning is significant for total cost, the profitability scenarios investigate which learning behavior the modular manufacturing should present to be competitive with respect to the conventional technology.

The base case and the profitability scenarios are bridged by a sensitivity analysis step. Conclusions from the initial cost performance analysis of the base case are used to determine which promising variables should be further analyzed. The sensitivity analysis step screens these variables and checks which ones should be considered in the profitability scenarios.

The steps of the developed modular TEA framework are briefly summarized in Figure 2. The requirements of this framework are knowledge about nominal operating points and process flow diagram topologies for the technologies to be compared. The application of these steps is recommended for analysis of modular systems that have undergone process synthesis and, if applicable, process operability analysis. Each step is discussed in detail in the following subsections. Subscripts *con*, *mod* and *MP* are associated with conventional plant, modular units and assembled modular plant, respectively.

3.1 | Capital cost estimation

In general, capital costs can be estimated by first calculating purchase cost at base conditions, followed by cost additions due to custom materials and operation, and

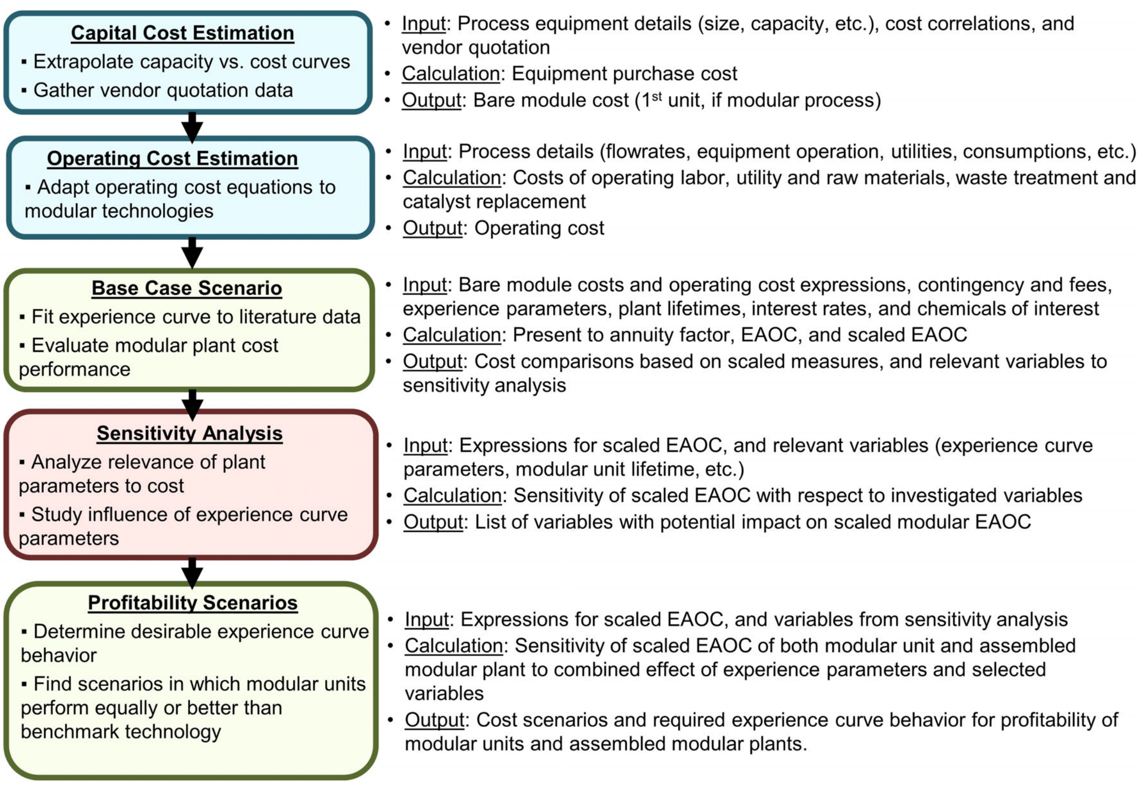

FIGURE 2 Summarized step-by-step modular TEA framework

finally by considering indirect costs, contingency, fees, and the presence of auxiliary facilities. The purchase cost is usually determined using process capacities (volume, diameter, area, power, flowrates, etc.), which are either associated with capacity vs. cost data or with the six-tenths rule.[14] Here, these methods are applied to estimate the capital cost of conventional and modular technologies. New adaptations are developed to extend the estimation methods to modular processes.

The modular equipment is approximated to the closest possible conventional equipment type. Then, the purchase cost calculation is performed by extrapolating capacity vs. cost curves beyond minimum reported sizes.[9] The consideration of custom conditions and other cost factors is replicated from the methodology for costing conventional plants. While an estimation of modular capital cost is enabled, this method provides an upper bound price estimate because lower equipment capacities tend to overprice modular equipment cost, when, in reality, modular design and production are expected to be faster, safer and cheaper.[4]

Alternatively, quotation data for modular technologies is recommended when available. Nevertheless, the generation of capacity vs. cost data is hindered due to the degree of customization of new modular technologies. As a solution, when single cost data points are available, the six-tenth rule can be applied.

Bare module costs are defined as capital costs that include purchase cost and all direct and indirect costs, but contingency and fees. These costs are estimated for both conventional and modular processes. When calculated, the conventional process presents a final value, represented by $C_{BM,con}$, because the economy of learning is reserved for the production of modular systems. The bare module cost estimation of the modular process, represented by $C_{BM,mod}$, is in turn associated only with the cost of the first produced modular unit. In this work, the costs of n^{th} manufactured modules are indicated by superscripts, and, therefore, the first modular unit presents $C^1_{BM,mod}$.

For subsequent modular units, assuming an experience curve described by Equation (1), the bare module cost can be estimated according to the level of maturity. In this case, Equation (3) is the result of adapting Equation (2) to the modular bare module cost case.

$$C^n_{BM,mod} = F_n \cdot C^1_{BM,mod} = (1 - R_n) \cdot C^1_{BM,mod} \tag{3}$$

where $C^n_{BM,mod}$ is the bare module cost of the n^{th} unit, F_n is the multiplier for cost reduction for the n^{th} modular unit, R_n is the actual cost reduction, and $C^1_{BM,mod}$ is the bare module cost of the first modular unit estimated above.

Another important consideration is related to values of contingency and fees. Typically, contingency and fees are lumped together and add about 3% and 15% to the total capital cost, respectively. Contingency represents reliability in cost data and completeness of the flowsheet.[14] In this framework, the sum of 18% for contingency and fees is assumed for conventional technologies as cost data is likely to be available. For modular systems, cost data is notably scarce, and, therefore, the usual value of contingency of 15% may not be realistic. Therefore, values of contingency above 15% are considered for modular cases. Equation (4) shows the total module cost, or fixed capital investment, calculated as a function of bare module and contingency and fees. If desired, new site development could be included by adopting the measure of grassroots roots cost,[14] which corresponds to an approximate increase of 50% to the bare module cost. The adoption of this estimation to modular systems can be done and, in that case, it would be considered a worst-case scenario, since modular plants have less requirements for space and land development.

$$C_{TM} = (1 + a) \cdot C_{BM} \tag{4}$$

where C_{TM} is the total module cost, a represents additional cost increase due to contingency and fees, and C_{BM} is the bare module cost.

In this step, the two values of bare module costs associated with the conventional process and first modular unit are calculated. Total module costs are estimated in the base case scenario, sensitivity analysis, and profitability scenarios, where experience parameters and values of contingency and fees are analyzed in more depth.

3.2 | Operating cost estimation

The operating cost includes direct costs, fixed costs, and general expenses. A detailed explanation of each of these terms correspond to the definition of "manufacturing costs" for traditional chemical process design costing from ref. [14]. Here, the term "operating cost" is chosen to establish distinction from the costs related to the manufacturing, or fabrication, of modular units. To systematically estimate the operating costs, the classification of operating costs as direct and indirect costs and general expenses is employed. These costs are in turn broken down as functions of the depreciation, fixed capital investment, operating labor, utilities, waste treatment and raw materials.[14] Here, conventional operating cost equations are adapted for an adequate comparison between modular and conventional technologies.

For process integrated modular systems, straightforward distinction between raw materials and utilities may be impaired. New modular technologies are also likely to count on advances in the field of novel catalysts, thereby making catalyst replacement play an important role in the modular operating cost. To account for these particularities, the operating cost equation from ref. [14] is modified. Raw materials and utilities are lumped in a single cost term, and the catalyst replacement cost is explicitly included as part of direct manufacturing costs. Note that these changes for raw materials/utilities are considered specifically to modular technologies in which raw materials are also utilities (in this case natural gas). As a result, Equation (5) describes the estimated annual cost of operation as follows:

$$COM = 0.280 \cdot C_{TM} + 2.73 \cdot C_{OL} + 1.23 \cdot (C_{URM} + C_{WT} + C_{CAT}) \tag{5}$$

where COM is the total operating cost; C_{TM} is the total module cost; C_{OL} is the cost of operating labor; C_{URM} refers to costs of utilities and raw materials; C_{WT} is the cost of waste treatment; and C_{CAT} is the cost of catalyst replacement. A depreciation of 10% of fixed capital investment was assumed. While this depreciation value is typically used for industrial-scale processes, it should provide a reasonable starting point estimation for modular systems.

For both modular and conventional technologies, total module costs are calculated using obtained values of bare module cost from the previous step and Equation (4). Here, the cost of operating labor is assumed to be the same as in a regular plant of similar scale. First, the cost of operating labor is estimated for the conventional technology, then it is linearly scaled for the modular unit using production capacities. Equation (6) corresponds to the estimation of modular operating labor cost.

$$C_{OL,mod} = \frac{T_{i,mod}}{T_{i,con}} \cdot C_{OL,con} \tag{6}$$

where C_{OL} refers to the costs of operating labor, $T_{i,con}$ and $T_{i,mod}$ correspond to productions of a chemical of interest of the conventional plant and modular unit, respectively. Note that the above assumption also provides an upper bound cost estimate, since modular systems are expected to be more autonomous and less staffed.[4] This assumption allows the estimation of operating cost, as there is a lack of estimation methods for costing modular operating labor in the available literature.

Stream flowrates of utilities, waste treatment, and raw materials are determined using process simulation if plant data is not available. The cost of raw materials is estimated using historical market values and projections. The costs of utilities and waste treatment are calculated either: (i) using reference tables, assuming that utility generation and waste treatment happen as in large-scale industries; or (ii) by synthesizing and costing modular equipment that perform those tasks.

Utilities bought at the plant's boundary limits such as water, air and power are likely not to be affected by modularization. However, generated utilities and treatments that require substations depend on the modularity considerations. The inclusion of modular substations results in a cost that is based on utilities (or raw materials) bought at the boundary limits, rather than a cost representation based on reference tables.

The outcomes of this step are the expressions for COM_{con} and COM_{mod} as functions of bare module cost, contingency, and, for the modular case, experience parameters and number of manufactured modules. The dependence of the operating cost functions with respect to these variables can be expressed as $COM_{con}(C_{TM,con}) = COM_{con}(C_{BM,con}, a_{con})$ and $COM_{mod}(C_{TM,mod}) = COM_{mod}\left(C^1_{BM,mod}, a_{mod}, \alpha, R_{max}, n\right)$.

3.3 | Base case scenario cost estimation

In this step, a base case scenario provides insights about the overall cost performance of the analyzed modular system in comparison with a benchmark technology of traditional scale. The objective in this study is to identify which influencing cost parameters should be further investigated using sensitivity analysis. Particularly, the relevance of the economy of learning is evidenced, indicating whether experience parameters should be further studied as well.

At first, experience parameters are estimated using literature data so that both COM_{con} and COM_{mod} can be calculated. Then, capital and operating costs are merged into a single $EAOC$ profitability indicator. Equation (7) below depicts the calculation of $EAOC$ by converting the capital costs to annuity.[14]

$$EAOC = C_{TM} \cdot PA + COM \tag{7}$$

where $EAOC$ is the equivalent annual operating cost, C_{TM} and COM follow the previous descriptions, and PA is the present to annuity factor. PA is a function of the plant lifetime and interest rate. Equation (8) shows how PA can be calculated.

$$PA = \frac{ir(1+ir)^{lf}}{(1+ir)^{lf} - 1} \tag{8}$$

where ir is the interest rate and lf is the plant lifetime.

The $EAOC$ is also scaled with respect to production of a chemical of interest so that the comparison can be performed independently of production scale. Equation (9) scales the $EAOC$ with respect to annual production of the chosen chemical.

$$EAOC' = \frac{EAOC}{T_i \cdot OP} \tag{9}$$

where $EAOC'$ is the scaled $EAOC$ in US\$/kg of chemical of interest, T_i refers to the production rate of a chemical of interest in kg/h and OP is the annual plant operating time in h/yr.

Finally, the scaled cost estimates are directly compared for the selection of variables that will be further investigated. The value of $EAOC'$ indicates which technology is more profitable given the employed parameters. Specific terms are scaled and compared to show possible bottlenecks of the modular technology. For example, cost of waste treatment can be scaled using $C_{WT}/(T_i \cdot OP)$ to show how significant this cost is for composition of the $EAOC'$.

3.4 | Sensitivity analysis

Screening of variables with a focus on economy of learning is performed through sensitivity analysis. Parameters with higher degree of uncertainty in modular deployment projects are investigated, including contingency, experience parameters, and modular unit lifetime. Other relevant cost variables may be included in case the cost performance from the previous step indicates potential. This step provides guidelines on which variables should be studied to find scenarios that are favorable to the modular technologies.

3.5 | Profitability scenarios

In this study, profitability is analyzed in two distinct cases: (i) a modular plant is constructed assuming fixed capital and operating costs, and the technology is evaluated at maturity; and/or (ii) a modular plant is scaled-up supposing bulk purchase of modular units at learning stage, and, therefore, consider a gradual decrease in costs due to the economy of learning. The first case indicates future competitiveness of the modular technology, whereas the second case analyzes profitability of the complete construction process, including higher initial costs of the first units.

This step consists of an extension of the sensitivity analysis to check in which conditions modular systems may present advantages over the conventional plant. As outcome, the first case shows what conditions of cost reductions are needed for competitiveness, independently of the experience rate exponent. The second case shows how the experience rate exponent can be included in the analysis by adopting a measure of profitability that comprises deployment and operation of several modular units that compose a modular plant with production rates equivalent to the conventional scale.

4 | APPLICATION PROCESS: MODULAR STEAM METHANE REFORMING

A modular hydrogen unit is considered for the application of the developed framework, in which the main focus is the costing of the modular unit. Intensification strategies are employed to provide enhanced heat transfer to the endothermic steam reforming reactions. The process model includes pretreatment, purification, and generation of power and steam. The modular unit operations are integrated to minimize consumption of utilities, aiming system self-sufficiency. Similar work has been done to address modeling and process intensification of similar application units.[17,18]

If deployed, modular SMR units could be applied to monetize unused NG resources. Shale gas consists of a geologically distributed NG source that can be recovered in short-term wells, and therefore require dynamic drilling and production. Landfill and associated gas in oil recovery are other examples of stranded NG, which are usually flared due to the lack of infrastructure for processing and utilization. NG in remote locations is another example of unrecovered gas linked to costly transportation and associated construction work (pipelines, etc.).

Transportability and cheaper maintenance costs are promising features to address the challenges of untapped NG. Intensified modular systems can also significantly decrease process footprint, reducing the requirements associated with groundwork and infrastructure. The proposed framework is applied to systematically evaluate economic feasibility of the considered modular hydrogen production unit. Modular profitability is studied with a focus on the comparison with existing large-scale SMR plants. In this section, process flowsheet development and operability analysis are initially presented, followed by the application of the modular TEA framework.

4.1 | Process development

The synthesis of the modular hydrogen unit starts with equipment that represent the most drastic changes. The remaining parts of the process are then designed by creating modular versions of the necessary unit operations to complete the flowsheet synthesis.

Initially, a microchannel reactor is considered as an intensified modular equipment that substitutes the conventional unit operations of pre-reforming, reforming furnace, and high-temperature shift. The microchannel reactor is scaled up from literature experimental data.[3] Figure 3 depicts a simplified schematic corresponding to the literature experimental design.[3]

In this process, NG undergoes combustion in the combustion microchannel. Then, the increased contact area between microchannels is responsible for enhanced heat transfer from the combustion microchannel to a reaction microchannel, where hydrogen production is facilitated by endothermic reactions. Particularly, the following reactions take place in the reaction microchannel:

$$CH_4 + H_2O \leftrightarrow CO + 3H_2 \tag{10}$$

$$CO + H_2O \leftrightarrow CO_2 + H_2 \tag{11}$$

$$CH_4 + 2H_2O \leftrightarrow CO_2 + 4H_2 \tag{12}$$

Equations (10)–(12) represent steam-methane reforming, water-gas shift and reverse methanation, respectively. The microchannels are filled with specific types of catalyst. Details on catalyst distribution and geometry of microchannels can be found in ref. [3].

Scale up is carried out for the design of a microchannel reactor using experimental data. As a result, about 3000 pairs of microchannels compose the design of a reactor that produces approximately 0.36 Sm^3/s of hydrogen corresponding to expected commercial performance.[3] Heat losses drop from 45% at experimental scale to less than 5% for the commercial scale design, as consequence of placing a high number of microchannels together in an optimal manner.[3] Subsection 4.2 below shows how operability analysis is employed to adjust the ratio between fuel and combustion fed to each type of microchannel.

Process synthesis is then performed to include unit operations of pretreatment of NG, steam production and hydrogen separation and purification. The NG first passes through desulphurization beds, where sulfur removal takes place. Then, it is mixed with steam, and converted to a mixture of hydrogen, carbon monoxide, carbon dioxide, steam, and unconverted methane in the microchannel reactor. Water is knocked out from the product stream and treated for reuse in the steam production boiler. Pressure swing adsorption (PSA) finalizes the process by separating about 90% of all produced hydrogen. Figure 4 shows a simplified block flow diagram of the proposed modular hydrogen unit.

The modular SMR process is modeled in Aspen Plus® Version 9.0. For the microchannel reactor model, combustion takes place in a stoichiometric reactor and reaction in a plug-flow reactor. Multipliers account for scaling-up and heat transfer follow a custom model in which a fraction of the produced heat is dissipated, and the remaining heat is transferred to the reaction microchannel.

Utility heat exchangers are initially placed for conditioning streams. Aspen Process Economic Analyzer is employed to integrate the heat exchangers and minimize utility usage. Figure 5 shows the final hydrogen unit process model in Aspen Plus. Details on model assumptions and specific flowrates can be found in Appendix A.

4.2 | Operability analysis

The experimental design of the microchannel reactor operates in accordance with a heat loss of about 45% as pointed out in Subsection 4.1. When scale up is completed, and the commercial scale design presents a heat loss of less than 5%, the heat production in the combustion microchannels must be regulated. Process operability analysis concepts are employed to determine a feasible microchannel reactor operation in which heat is generated according to reaction needs.[5,15] The flowrates of NG as fuel, NG as feedstock and steam are systematically changed to regulate the production of heat and the consumption by endothermic reaction. Although the operability analysis focuses on the operation of the microchannel reactor, input and output variables associated with the entire unit are selected.

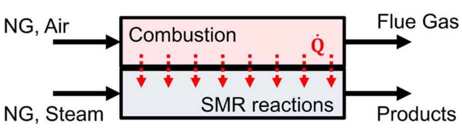

FIGURE 3 Experimental scheme of consecutive microchannels

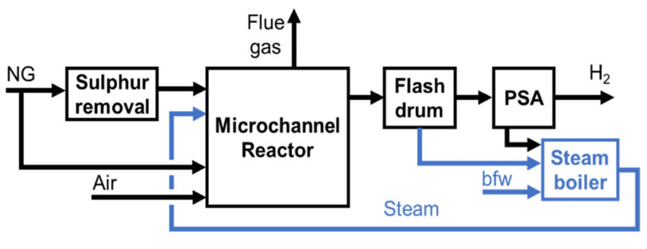

FIGURE 4 Simplified block flow diagram: Modular hydrogen unit

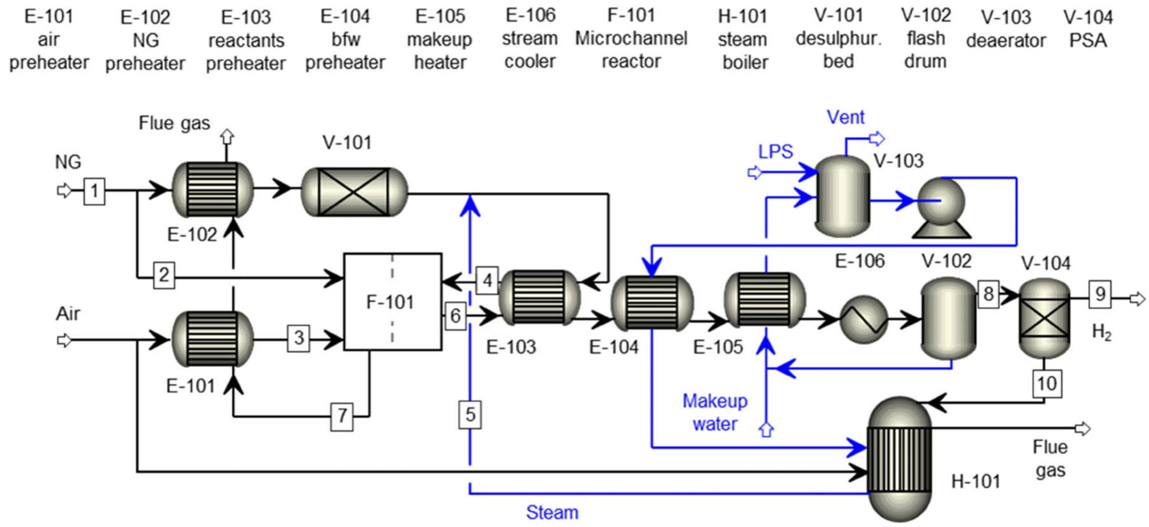

FIGURE 5 Process flow diagram: Modular hydrogen unit (adapted from Aspen plus)

The described process model is integrated with MATLAB for the operability analysis using the Process Operability App.[19] ActiveX automation server is used to allow a MATLAB script to open, change variables, simulate, collect results, and register logs from the Aspen Plus simulations. For this application, the selected manipulated variables (MVs) are the NG flowrate directed to reaction microchannels, NG flowrate directed to combustion microchannels and steam to carbon ratio. The controlled variables (CVs) are methane conversion, hydrogen flowrate to unit's boundary limit (BL) and required heat efficiency. A MATLAB script is written to change MVs and collect CVs after the simulations are run.

The expected ranges in which MVs are changed compose the available input set (AIS) for operability analysis. The simulations of all operating points define the achievable output set (AOS) for the analysis. The ranges of NG flowrate sent to reaction microchannels and steam to carbon ratio are based on reported values from the experimental microchannels.[3] The range of NG flowrate employed as fuel is determined by adopting a typical experimental value as upper bound and a value close to zero as lower bound since fuel usage decreases with the scale up due to reduction in heat losses.

The desired ranges of CVs describe the desired output set (DOS) for operability. For this set, methane conversion experimental values are assumed as the lower limit and the maximum mathematically possible conversion (100%) as the upper limit. Similarly, desired amounts of produced hydrogen have their lower and upper limits determined by reported experimental performance and maximum production assuming full methane conversion. The required heat efficiency is defined as the complement of heat loss, and, as the heat loss is expected to be lower than 5%, the required heat efficiency should be above 95%. Tables 1 and 2 contain the adopted ranges for AIS and DOS sets.

The composition of NG is considered as a system disturbance. For the selection of nominal design and operation, NG is assumed to be at a nominal point, that is, there is no perturbation. An average between the methane concentration of 95.8% from the experimental microchannel design and typical methane concentrations of at least 99.3% for pipeline quality is adopted.[3,20] Therefore, the nominal NG composition is defined as 97.56% for the methane concentration in mol_{CH_4}/mol_{NG}.

Operability algorithms are run to find the combinations of MVs that achieve the described DOS. Particularly, multimodel algorithms are adapted to include interpolations and better define the resulting regions.[19] Figure 6 shows the AIS and calculated feasible operating region. Figure 7 shows the AOS, the DOS and their intersection, which determines the feasible operating region.

In these figures, the feasible operating region is approximated by parallelepipeds and the nominal operation is assumed to be the point in the center of that region. The selected nominal operation is defined by NG flowrates to reaction and combustion microchannels of 17.15 kmol/h and 5.52 kmol/h respectively, and steam to

TABLE 1 Manipulated variables and available ranges

Manipulated variable	Available range
NG - SMR (kmol/h)	16.46–17.24
NG - fuel (kmol/h)	0.50–9.52
Steam to carbon ratio (–)	3.0–4.8

TABLE 2 Controlled variables and desired ranges

Controlled variable	Desired range
CH_4 conversion (%)	92.48–100
Hydrogen to BL (Sm^3/s)	0.32–0.41
Required heat efficiency (%)	95–100

carbon ratio of 4.76. This nominal point takes the CVs to assume the values of 92.57% for methane conversion, 0.32 Sm^3/s for final hydrogen production, and 96.56% required heat efficiency. Note that the chosen MVs take the CVs inside the designed DOS.

Finally, using the nominal point, the entire plant is checked for possible constraint violation and compliance with specified temperatures. Heat exchanger areas are further adjusted when needed using design mode of Aspen Plus to accommodate the change from experimental to commercial scale operation of the microchannel reactor.

4.3 | Application of the modular tea framework

A conventional SMR hydrogen plant that produces 29.5 Sm^3/s of hydrogen is adopted as a benchmark technology for the application of the modular TEA framework. The conventional SMR presents regular equipment sizes and noticeable differences to the modular unit. Besides converting methane through several unit operations, a reactive furnace provides excess heat that is used for steam production. The considered SMR flowsheet is based on ref. [21], where specific details regarding the process flow diagram and flowrates can be found. Figure 8 shows the simplified flow diagram of the conventional SMR plant. Alternatively, if a SMR process installed in a different location was adopted, the number of required modular units that are needed to achieve the specified production rate would change according to that corresponding location.

Considering the obtained modular unit and the adopted conventional counterpart, the same steps from Section 3 are applied in the following subsections. For fairness, same cost techniques and assumptions are performed for both modular and conventional systems whenever possible.

4.3.1 | Capital cost estimation

For the considered benchmark SMR plant, capital cost is obtained through adjustments using reported values.[21] After inclusion of location factor and currency adjustments, the bare module cost of the considered SMR plant is about $C_{BM,con} = \text{US\$}\,78,300,000$.[22]

The capital cost of the modular hydrogen unit is estimated by combining the two techniques described in Subsection 3.1. For most modular equipment, the capital cost is obtained from conventional equipment approximation and extrapolation of capacity vs. cost curves. For equipment associated with PSA, desulfurization and deaeration, modular processes from the literature are scaled using the six-tenths rule.

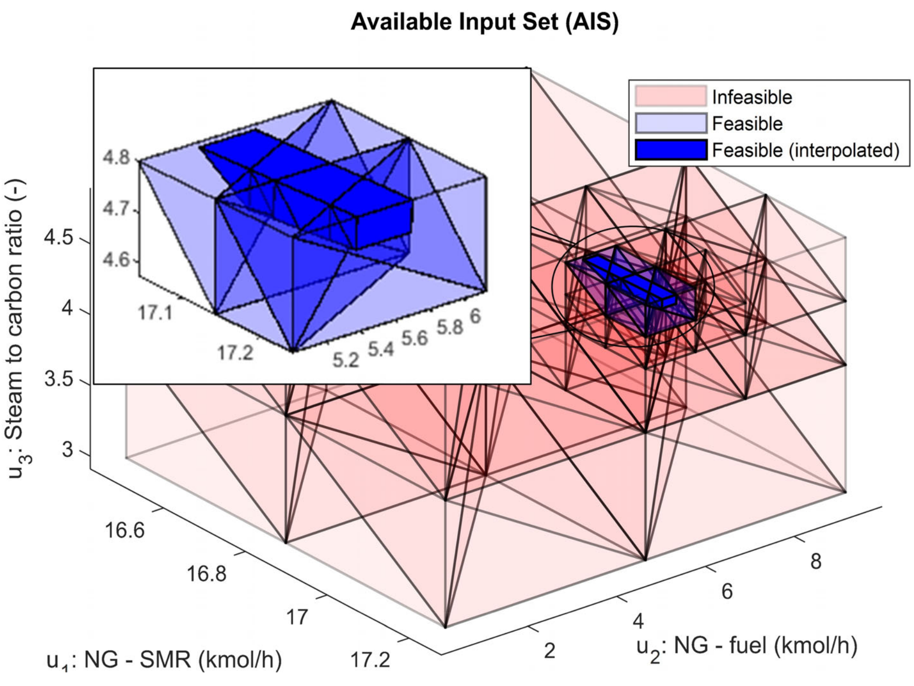

FIGURE 6 AIS and feasible operating input region

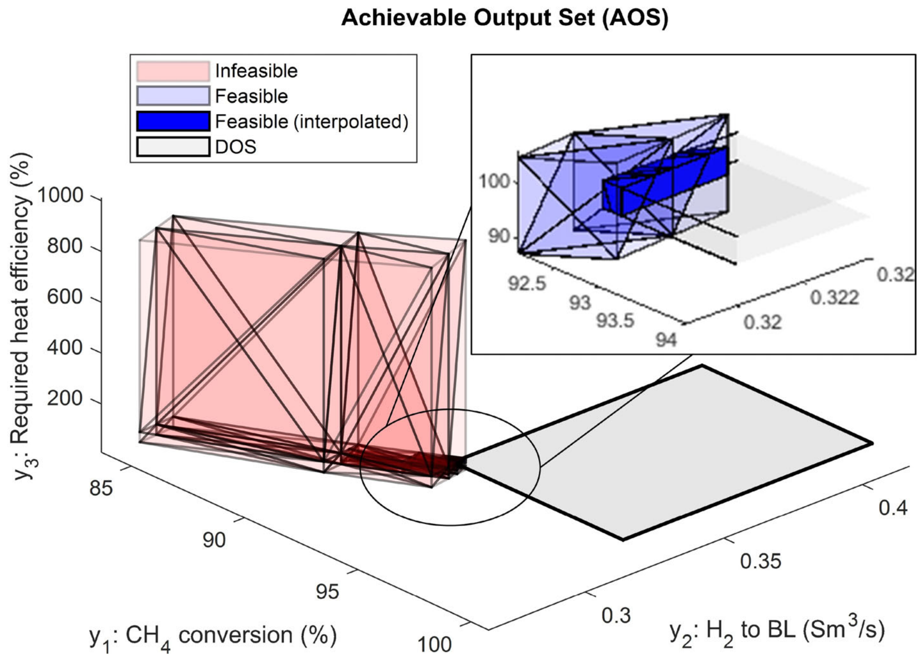

FIGURE 7 AOS, DOS and feasible operating output region

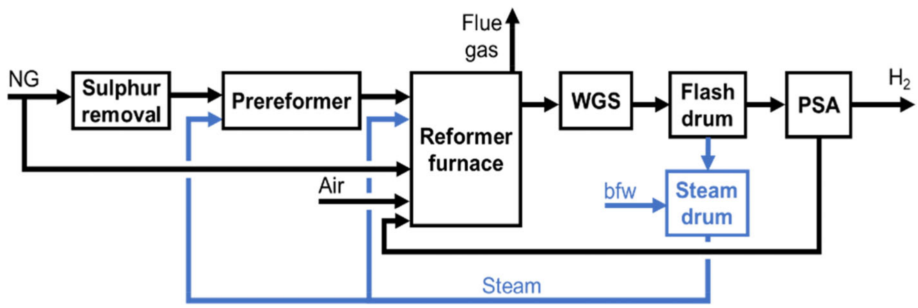

FIGURE 8 Simplified block flow diagram: Conventional SMR plant

For the approximation of modular equipment as conventional, all the heat exchangers are considered as shell and tube of floating head type; the microchannel reactor as a reformer furnace; the boiler as a conventional steam boiler; and the flash drum as a vessel. To extrapolate the capacity vs. cost curves associated with each type of equipment, the methodology from ref. [14] is repeated, but allowing for the estimation of purchase cost to be calculated outside of expected limits when needed. Factors associated with design pressure, materials of construction and other indirect costs are included to convert the purchase cost estimation into bare module cost estimations.

The PSA and desulfurization beds have their purchase cost scaled using modular equipment literature data from ref. [23]. The six-tenths rule is applied with total feed mass flowrate as attribute. Then, the bare module costs are estimated by considering the pieces of equipment as process vessels. The same procedure is used to cost the deaerator but using data associated with regular-scale deaerators.

Table 3 includes the calculated bare module costs of the modular equipment considered in the modular hydrogen unit. The process flow diagram nomenclature from Figure 5 is also adopted here. Details on individual cost calculation (material, design conditions, purchase cost, etc.) can be found in Appendix B.

In Table 3, $C^1_{BM,mod} = \text{US\$}\,3{,}599{,}075$ is the sum of all individual bare cost module costs and consists of the total bare module cost estimation for the first modular unit. The scale of this modular unit is associated with the nominal operation obtained in Subsection 4.2 and corresponds to a hydrogen production of about 0.32 Sm^3/s. Note the differences in scale and cost: the modular unit has a hydrogen production and a bare module cost of 0.32 Sm^3/s and about US$3600000, respectively, whereas the benchmark plant presents values of 29.5 Sm^3/s and US$78300000, respectively. The obtained values of bare module cost will be employed for calculation of total modules costs, operating costs and scaled economic measures.

TABLE 3 Estimated modular bare module cost

Id.	Scaling attribute	Bare module cost
E-101	Area, 29.5 m^2	US$ 160 366
E-102	Area, 22.5 m^2	US$ 162 922
E-103	Area, 71.7 m^2	US$ 198 737
E-104	Area, 19.2 m^2	US$ 163 205
E-105	Area, 1.2 m^2	US$ 517 480
E-106	Area, 15.4 m^2	US$ 163 965
F-101	Duty, 1050 kW	US$ 682 216
H-101	Duty, 830 kW	US$ 851 823
V-101	Inlet flowrate, 285 kg/h	US$ 153 794
V-102	Volume, 0.007 m^3	US$ 11 854
V-103	Inlet flowrate, 1630 kg/h	US$ 14 064
V-104	Inlet flowrate, 716 kg/h	US$ 518 649
$C^1_{BM,mod}$		US$ 3 599 075

4.3.2 | Operating cost estimation

For both SMR processes, total module costs remain a function of bare module costs and contingency. The total module cost for the modular hydrogen unit is also dependent on experience parameters and number of manufactured modules. As a result, the total module costs are expressed as $C_{TM,con} = C_{TM,con}(C_{BM,con}, a_{con})$ and $C_{TM,mod} = C_{TM,mod}(C^1_{BM,mod}, a_{mod}, \alpha, R_{max}, n)$. The values that allow for estimation of total module costs are explored in the following subsections.

The conventional plant has its cost of operating labor, $C_{OL,con}$, estimated considering that 22 operators are required for the operation of the hydrogen unit alone. The considered wage of an operator is the annual mean wage in chemical plants located in WV, in the range of the Marcellus Shale formation – a shale gas formation that would benefit from dynamic modular NG utilization.[24] Table 4 shows the considered annual wage along with prices adopted in the operating cost estimation such as raw materials, utilities, electricity and so on.

$C_{OL,mod}$ is then estimated using Equation (6). The hydrogen productions of 29.5 Sm^3/s for the conventional SMR and 0.32 Sm^3/s for the modular unit are converted to mass flow and assigned to as productions of the chemical of interest $T_{H_2,con}$ and $T_{H_2,mod}$, respectively.

The cost of utilities and raw materials is comprised of the costs of air, cooling water, NG, and steam. The costs of air, cooling water and NG are determined by considering the respective flowrates in each process. The cost of steam, however, is estimated not only by accounting for the direct intake of chemicals, but also by calculating indirect consumptions such as power and circulating water treatment. To estimate the cost of steam, the costs of heating, treating and circulating water, air blowing, makeup boiler feedwater, and pumping boiler feedwater are considered. An electricity credit is applied to compensate for the presence of a steam turbine.

For the conventional SMR, the cost of heating can be neglected, since enough heat is supplied from the process streams and SMR furnace, which is fueled by PSA tail gas and NG–already considered. The costs of treating and circulating water, air blowing, and pumping are estimated using mass flowrates obtained from balances in the reference plant. Electricity credit is estimated using reported power production.

For the modular unit, the cost of heating is also neglected because process heat is used to preheat boiler feedwater and the steam boiler is fueled solely by PSA tail gas. The costs of treating and circulating water and air blowing are estimated using the mass flowrates from the Aspen Plus simulation. Pumping cost and electricity credit are calculated using simulation values of pump net power and excess of heat from the steam boiler. For the latter, a turbine that presents 90% of thermal efficiency is considered.

The cost of waste treatment is simplified to the cost of wastewater treatment. For both processes, a unit for secondary wastewater treatment is considered available. Most of the wastewater is assumed to come from a blowdown or water purge, which is estimated to be about 10% of all circulated water.

Catalyst is considered for both cases, assuming yearly replacement. For the conventional SMR, reference values are employed. Whereas, for the modular hydrogen plant, the presence of catalysts is considered inside the microchannel reactor, for combustion and various SMR

TABLE 4 Adopted market values

Item	Value
Natural gas	US$ 0.1119/Sm^3
Air	US$ 0.5/100 Sm^3
Cooling water	US$ 15.7/1000 kg
Wastewater treatment	US$ 43/1000 kg
Circulating water treatment	US$ 0.156/1000 kg
Electricity	US$ 0.0674/kWh
High-purity water for process use	US$ 0.177/1000 kg
Microchannel reactor catalyst	US$ 0.2206/pair of microchannels
Desulfurization catalyst	US$ 355/ft^3
Average operator wage	US$ 67 350

reactions, and desulfurization unit. Both technologies leave catalyst replacement of PSA units out.

The outcome of this step are values for the expressions $COM_{con}(C_{BM,con}, a_{con})$ and $COM_{mod}(C^1_{BM,mod}, a_{mod}, \alpha, R_{max}, n)$. Assumptions regarding contingencies and experience curve are further studied in the following subsections for analysis of profitability.

4.3.3 | Base case scenario

The experience curve is fitted to literature values that indicate a maximum price decrease of around 42% at the 10th produced modular unit.[12] Using Equation (1), R_{max} is fixed at 42% and α is varied to reduce the mean square error between literature data points and model data points. Literature data is taken from ref. [12] and refers to construction of modular nuclear reactors. Note that other base cases could also be considered for characterizing the experience curve.[25] Figure 9 shows both data points from the literature and the obtained model values. The experience rate exponent that minimized the mean square error is $\alpha = 0.24$, and along with $R_{max} = 42\%$ defines a base case economy of learning for modular systems.

Using the modeled experience curve and above results, total module and operating costs are calculated along with scaled economic measures. For the base case scenario, the technology maturity is assumed for modular units. Therefore, values of $n \geq 10$ are considered, providing constant results for the $C_{TM,mod}$ and COM_{mod} calculations.

For both technologies, the following cost assumptions are considered:

- Standard of 18% for contingency and fees ($a_{con} = a_{mod} = 18\%$)
- Plant lifetime of 25 years ($lf_{con} = lf_{mod} = 25\,\text{yr}$)
- Interest rate of 6% per annum ($ir_{con} = ir_{mod} = 6\%$ per annum)

Then, comparison of scaled *EAOC* and its specific scaled terms, $C_{TM} \cdot PA$ and *COM*, is performed. Figure 10 contains the three economic measures. While the conventional SMR presents a scaled *EAOC* of about $1.3\,\text{US\$/kg}_{H_2}$, scaled annuitized capital cost of $0.1\,\text{US\$/kg}_{H_2}$ and scaled operating cost of $1.2\,\text{US\$/kg}_{H_2}$, the modular unit has values of $1.9\,\text{US\$/kg}_{H_2}$, $0.24\,\text{US\$/kg}_{H_2}$ and $1.7\,\text{US\$/kg}_{H_2}$, respectively. This result indicates a trend of the modular unit to present a higher overall hydrogen cost due to both capital and operating costs.

As modular intensified technologies are expected to have better efficiencies, the scaled operating costs are further detailed using the following terms: (i) depreciation, maintenance and repairs, operating supplies and other operating costs that depend on total capital cost, which are represented by $COM(C_{TM}) = 0.280 \cdot C_{TM}$; (ii) the operating labor, represented by $2.73 \cdot C_{OL}$; and (iii) specific terms associated with raw materials, utilities, waste treatment and catalyst replacement, which are represented by $1.23 \cdot C_i$, where C_i refers to each of the specific costs. These terms are scaled and illustrated in Figure 11.

In Figure 11, the main differences in operating costs are due to the terms associated with capital cost, $COM(C_{TM})$. Identical scaled costs of operating labor are a direct result of assumptions adopted using Equation (6). A slightly higher consumption of air is identified in the modular unit, mainly because of the occurrence of combustion in two unit operations consisting of a microchannel reactor and steam boiler as opposed to just one in the conventional process, the reforming furnace. The increased NG intake in the modular unit is a consequence of fueling the combustion microchannel with just methane. A lower steam cost in indicated for the modular unit, which is caused by a relatively higher production of

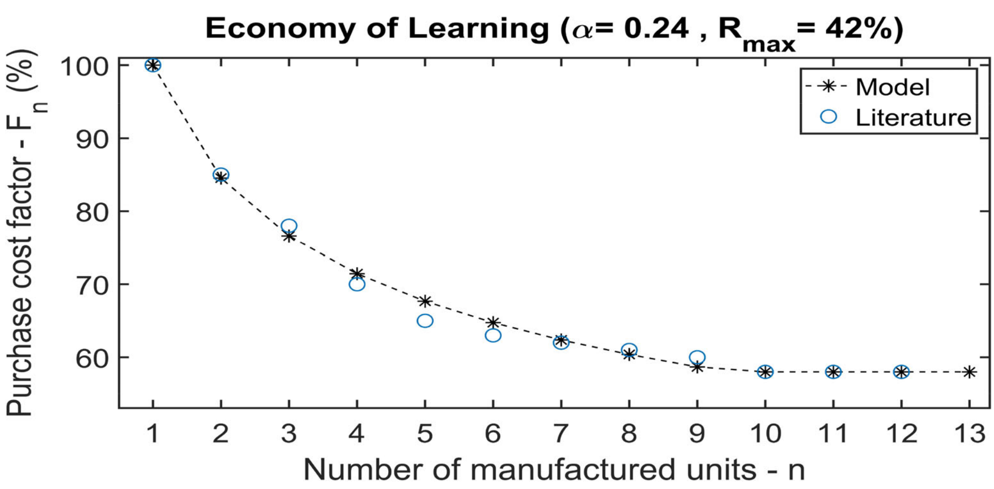

FIGURE 9 Experience curve: Model fitting. Literature data points taken from ref. [11]

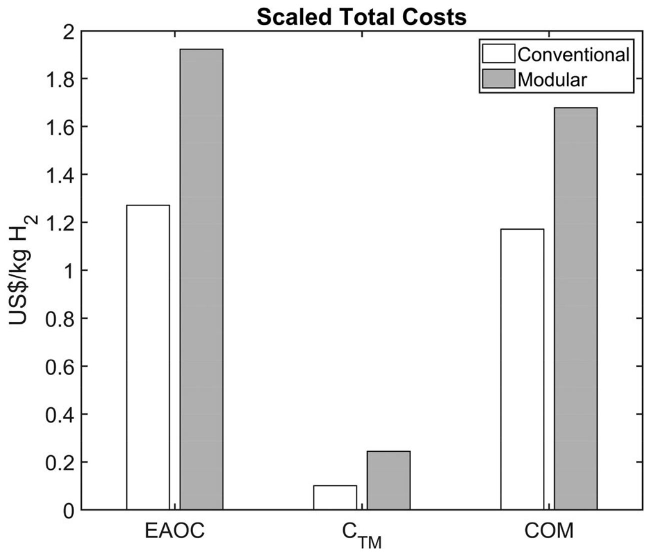

FIGURE 10 Comparison of scaled costs: EAOC, total capital cost and operating cost

electricity. The magnitude of the costs in Figure 11 indicates that terms associated with capital cost and cost of NG are the most significant factors for increasing the cost of hydrogen for the modular system.

Because capital cost is relevant in this comparison, experience parameters, modular contingency and fees, interest rate, and lifetime should be further investigated. Differences in cost of air, cooling water, water treatment and catalyst are slim and low in magnitude when compared to NG costs. As variations in price of NG are prone to happen in certain scenarios–particularly where natural is currently flared, NG price is also considered for further investigation.

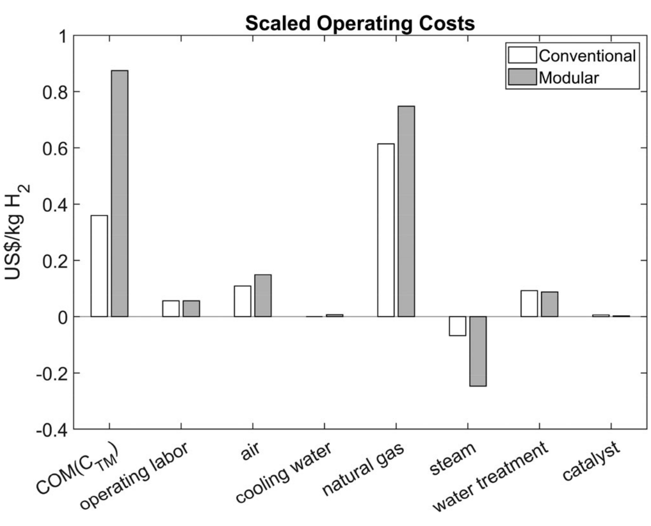

FIGURE 11 Detailed comparison of scaled operating costs

4.3.4 | Sensitivity analysis

Here, potential improvements in the scaled *EAOC* of the modular hydrogen unit are analyzed. Investigated variables are changed within an expected range, while other parameters are all held at the values described in Subsection 4.3.3. The sensitivity of the scaled modular *EAOC* is studied with respect to purchase cost reduction due to economy of learning (R_n), modular project contingency and fees (a_{mod}), modular unit lifetime (lf_{mod}), interest rate of the modular project (ir_{mod}) and price of NG where the modular unit is operated ($P_{NG,mod}$).

For the economy of learning, variation in the experience rate exponent, α, can only be accurately investigated in conjunction with the analyzed number of manufactured modular units and maximum reduction in cost, R_{max}. The simplification to purchase cost reduction R_n is adopted as alternative to the study of the 3 experience parameters. Values of R_n are the reduction in purchase cost observed for the entire experience curve, representing either cost reductions during the learning phase or R_{max} at technology maturity. For the sensitivity, R_n is tested within the range of 20–90%.

Regarding other variables, modular unit lifetime is analyzed within a range in which the lower bound of 5 years corresponds to a relatively low lifetime for a chemical plant, and the upper bound of 60 years corresponds to longer lifetimes, based in extreme cases such as nuclear modular reactors. The contingency and fees range is based on the expectation of contingency between 15% and 55% for technologies that follow an experience curve.[12] Supposing changes in fees from fiscal incentives, the minimum value for modular contingency and fees, a_{mod}, is at 15% and maximum, 58%.

Similarly, the interest rate is varied between 1 and 10% per annum (p.a.), corresponding to situations of low and high interests. NG price is analyzed for situations in which it is bought close to its market value and situations in which price declines due to stranded locations. For the first situation, the NG price upper bound is rounded up to US$ 0.012/Sm^3, based on the price depicted in Table 4. For the lower bound, free NG is considered. For none of the investigated parameters, financial stimulus–which would turn certain costs into credits, is considered.

All system parameters are held at the values described in Subsection 4.3.3. Then R_n, a_{mod}, lf_{mod}, ir_{mod}, and $P_{NG,mod}$ are changed individually within the expected ranges described above. The changes in scaled *EAOC* are monitored as each variable is changed. As a result, a sensitivity curve is obtained for each parameter: R_n, a_{mod}, lf_{mod}, $P_{NG,mod}$ and ir_{mod} vs. scaled *EAOC*. Figure 12 shows each of these curves. The base case values from Subsection 4.3.3. are represented as data points in the respective sensitivity curve for each analyzed variable. The scaled *EAOC* values corresponding to both modular and conventional technologies are included as horizontal lines.

The price of NG and reduction due to economy of learning display higher impacts on the *EAOC*. Price of NG alone presents potential to bring the modular unit to break-even scenarios when significantly decreased. The economy of learning, however, requires reductions of above 75% in purchase cost to do the same, which may not be realistic.

Contingency and fees come next in order of relevance. Higher values of contingency and fees may drift the modular technology away from competitive scenarios, if not compensated by other variables. Interest rate changes from the base case are insufficient to cause significant influence on final cost. Modular unit lifetime only plays a relevant role to around 18 years.

The assumption that a modular unit has a lifetime of at least 18 years is thus adopted. Therefore, both lifetime and interest rate are ruled out of further analysis. The combined effect of cost reduction due to the economy of learning, price of NG and contingency and fees is studied next. The following step analyzes cases in which these three variables are changes simultaneously for competitiveness of the modular process.

4.3.5 | Profitability scenarios

Case (i): Profitability of a modular hydrogen unit

The first profitability case is associated with individual modular units. NG price, contingency and fees, and price reduction due to economy of learning have their combined effect mapped to profitability scenarios. The variables are changed within the same ranges as in Subsection 4.3.4.

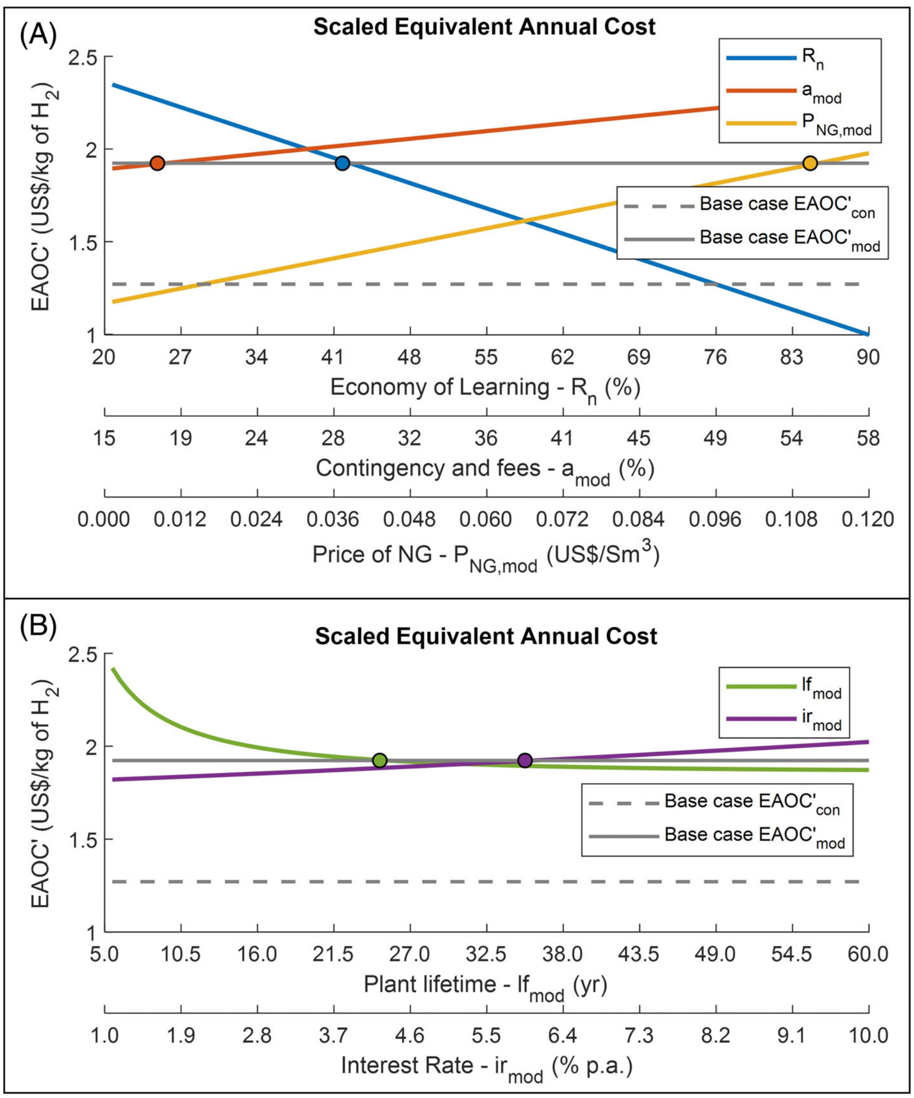

FIGURE 12 Sensitivity analysis of scaled *EAOC* of modular unit: (A) R_n, a_{mod} and $P_{NG,mod}$ and (B) lf_{mod} and ir_{mod}

The addressed scenarios aim to achieve break-even scaled *EAOC* and more aggressive reductions in price in comparison with the conventional SMR. Thus, the variables $P_{NG,mod}$, a_{mod} and R_n are mapped to $EAOC'_{mod}$. The studied profitability scenarios correspond to the following:

- Break-even cost of hydrogen: $EAOC'_{mod} = EAOC'_{con}$
- Reduction of 25% in cost of hydrogen for the modular case: $EAOC'_{mod} = 75\% \cdot EAOC'_{con}$
- Reduction of 50% in cost of hydrogen for the modular case: $EAOC'_{mod} = 50\% \cdot EAOC'_{con}$
- Reduction of 75% in cost of hydrogen for the modular case: $EAOC'_{mod} = 25\% \cdot EAOC'_{con}$

Combinations of $P_{NG,mod}$, a_{mod} and R that map to each scenario consist of a set in $\mathbb{R}^3$ that maps to a value in $\mathbb{R}$, corresponding to the aimed profitability scenario. To find a representation of those sets, Equation (9) is further developed for the modular unit. By substituting $C^n_{BM,mod}$, $C_{TM,mod}$, COM_{mod} and $EAOC_{mod}$, by Equations (3), (4), (5) and (7), respectively, setting the cost of NG expression apart from the cost of other utilities/raw materials, Equation (13) is obtained.

$$EAOC'_{mod} = \frac{(1+a_{mod}) \cdot (1-R_n) \cdot C^1_{BM,mod} \cdot (PA + 0.280) + 2.73 \cdot C_{OL,mod} + 1.23 \cdot (P_{NG,mod} \cdot V_{NG,mod} + X)}{P_{H_2,mod} \cdot OP} \quad (13)$$

where $X = \widetilde{C}_{URM} + C_{WT,mod} + C_{CAT,mod}$ corresponds to the sum of $\widetilde{C}_{URM}$, which is the cost of utilities and raw materials, excluding the cost of NG; $C_{WT,mod}$ is the cost of waste treatment; and $C_{CAT,mod}$ is the catalyst replacement cost.

The modular unit is analyzed for a nominal operation and a certain design. Thus, bare module cost and variables associated with operating cost are fixed. Supposing cases for which a_{mod} is fixed at particular values, Equation (13) can be interpreted as a linear equation of the following type:

$$EAOC'_{mod} = K_1 \cdot R_n + K_2 \cdot P_{NG,mod} + K_3 \quad (14)$$

where K_1, K_2 and K_3 are constants that depend on the adopted value of contingency and fees.

Contingency and fees are divided into a set that represents the extreme cases, that is, $a_{mod} \in \{15\%, 18\%, 58\%\}$. Then, for each case, four points of the complete economic model are simulated and values of K_1, K_2 and K_3 are found. The range of $P_{NG,mod}$ is divided into 100 points, $EAOC'_{mod}$ is set to a target value, and Equation (14) is solved for R_n. As a result, if achievable, combinations of R_n and $P_{NG,mod}$ that result in the target $EAOC'_{mod}$, given a_{mod}, are obtained.

This procedure is repeated for each a_{mod} and each profitability scenario. The results are plotted in Figure 13, in which each color represents a different profitability scenario.

Figure 13 indicates that NG price is the most decisive factor for economic feasibility of the modular hydrogen unit. The considered NG market value of US\$ 0.1119/Sm^3 is indicated by a vertical line related to the base case. The horizontal line indicates $R_n = 42\%$ from the base case. For NG at market value, a purchase cost reduction due economy of learning between around 77% and 83% is required, depending on the contingency and fees. Even with low fees and high reliability on cost data, the required reductions seem unrealistic.

The break-even and 75% of $EAOC'_{con}$ scenarios display potential when NG price decreases below 0.02 US\$/m^3. In this case, required reductions in purchase cost due to economy of learning are lower and approach the base case reference of 42%, implying that the modular unit can become competitive and slightly more profitable. More aggressive scenarios are likely to be unattainable because they require not only lower NG prices, but also higher reductions in purchase cost. The most aggressive scenario is of 25% of $EAOC'_{con}$ and would also require no fees and/or standard values of contingency, which is only observed in well-known technologies. For such scenario, values of a_{mod} of 15% and 18% are superimposed, while a_{mod} of 58% makes the goal of 25% of $EAOC'_{con}$ unachievable.

There is a tradeoff between contingency and fees and required R_n, suggesting that increase in reliability of flowsheet completion and modular cost data may result in more profitability. Naturally, first-of-a-kind modular designs should be associated with the upper cost situation, where $a_{mod} = 58\%$. Similarly, modular designs at maturity would be associated with lower cost situations, where a_{mod} approaches 15% without fees and 18% for standard fees of 3%.

This study indicates that the developed modular hydrogen unit competes with the conventional SMR only when NG prices fall below 0.02 US\$/Sm^3. Placement of

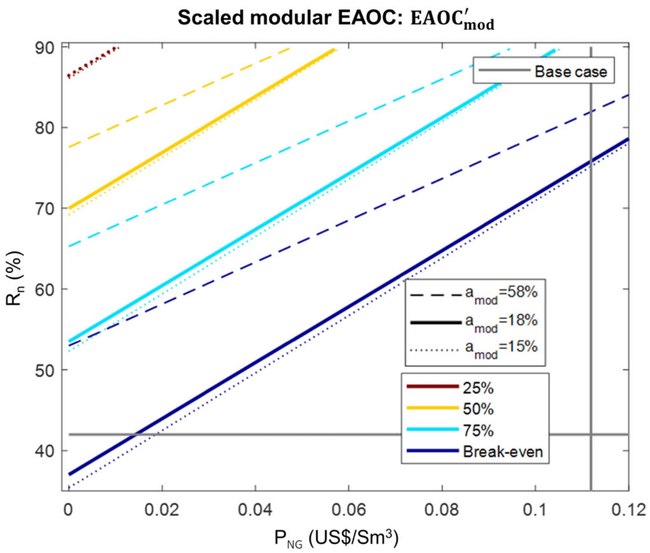

FIGURE 13 Achievability of profitability scenarios. Gray lines represent values from base case

modular hydrogen units where NG is abundant (remote locations and/or where flared occurs) would describe the situation in which NG price is low for the modular technology but is at market value for the regular plant, which is installed where infrastructure is more robust and NG demand is higher. The economy of learning suggests that the modular technology has potential to be more profitable as it approaches maturity. The effects of both reduction in price due to accrued knowledge and reliability in cost data and flowsheet development play in favor of the modular technology.

Case (ii): Profitability of a modular hydrogen plant

The bulk or massive purchase of modular units is studied to link the experience curve phenomena with modular deployment. The modular hydrogen units are placed in parallel to produce the same amount of hydrogen as the considered conventional SMR plant. Bulk purchase is assumed, and the units should start-up at the same time at a standard nominal operation. The cost model must be adapted to accommodate purchase costs that change with the experience curve.

The capital and operating costs are adapted to include differences between each purchased modular unit. Equation (4) is modified to represent the cost of the entire modular plant rather than the total cost of a modular unit. Equation (15) contains the total module cost expression for the modular plant. It is assumed that all units present the same value of contingency and fees.

$$C_{TM,MP} = (1 + a_{mod}) \cdot C^1_{BM,mod} \sum_{i=1}^{n} F_i \qquad (15)$$

where $C_{TM,MP}$ is the total module cost of the modular plant, a_{mod} are the contingency and fees, $C^1_{BM,mod}$ is the bare module cost of the first hydrogen unit, F_i is the multiplier for cost reduction for each ith modular unit, and n is the total number of purchased modular units.

Equation (5) is modified for calculation of the operating costs. Assuming all units operate at the same nominal point, Equation (16) shows the operating cost of the entire modular plant.

$$COM_{MP} = 0.280 \cdot C_{TM,MP} + n \cdot [2.73 \cdot C_{OL} + 1.23 \cdot (C_{URM} + C_{WT} + C_{CAT})] \qquad (16)$$

in which COM_{MP} is the operating cost of the modular plant, $C_{TM,MP}$ is the total module cost, n is the total number of purchased modular units, and the other variables follow the notation of Equation (5) and refer to the operation of an individual unit.

Equations (15) and (16) are then used for estimation of capital and operating costs. Then, Equations (7), (8) and (9) are applied for calculation of the scaled *EAOC* for the modular hydrogen plant.

The number of purchased units is calculated considering the productions of hydrogen of a modular unit and conventional SMR. As a result, a total of 92 modular units composes the modular hydrogen plant. This modular plant achieves a similar production of hydrogen as the conventional plant, which consists of 29.55 Sm^3/s.

The scaled *EAOC* for the modular plant is contrasted with the scaled *EAOC* of individual modular units. Assuming an experience rate exponent of $\alpha = 0.15$, maturity at $R_{max} = 40\%$ and free NG, the values of scaled *EAOC* are calculated for the first 100 modular units, and, thus, for modular plants that contain a total number of units that range from 1 to 100. Figure 14 explores the differences between the two scaled *EAOC* curves. The curve associated with the modular units represents the scaled *EAOC* for individual units. For example, the 22nd and 30th produced units have scaled costs of 1.27 and 1.21 US $/kg H_2, respectively. The curve associated with the scaled *EAOC* for the modular plant represents the cumulative cost of the assembled plant with a given number of units. For example, a modular plant that is bulk purchased and contains the first 22 modular units costs about 1.46 US$/kg H_2. Similarly, a modular plant that assembles the first 30 modular units has a total of 1.4 US $/kg H_2.

The trend from Figure 14 shows that, in general, for the adopted parameters, the modular units achieve break-even faster, at around the 21st produced modular unit. For the modular plant, however, break-even only

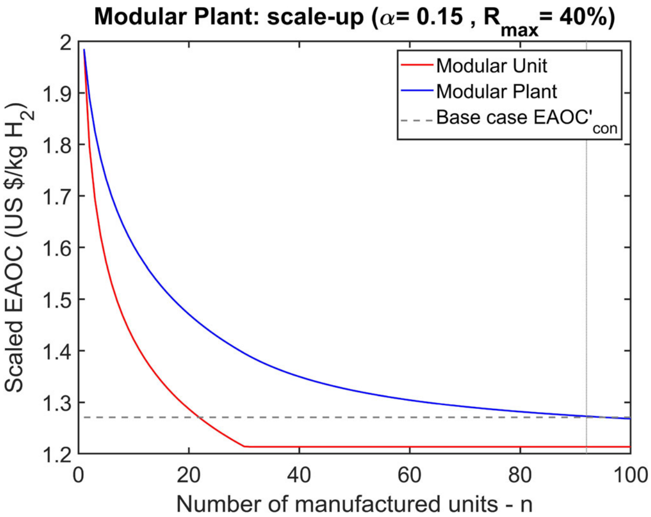

FIGURE 14 Differences between scaled EAOC of a unit and of the plant (cumulative) – $P_{NG} = 0\,\text{US\$/Sm}^3$. Dotted faded lines correspond to the number of units 92, required to achieve regular hydrogen production

occurs when the modular plant has around 90 modules. This happens because the price reduction from the second and subsequent modular units compensates for the higher purchase costs at the beginning of the learning process.

Values of α and R_{max} that provide break-even cost for the modular plant are determined. Two extreme scenarios of NG price are considered: free NG and market value. The scaled *EAOC* function is written as a function of NG price, α and R_{max}. The 100 points are obtained by discretizing the entire range of α. Finally, for each NG price scenario, each point is solved to obtain the value of R_{max} that provides break even, or $EAOC'_{con}$, given α.

The MATLAB subroutine *lsqnonlin* is employed to find each value R_n, which corresponds to a nonlinear least-squares optimization problem. The minimized objective function is set as the difference $EAOC'_{MP} - EAOC'_{con}$, in which $EAOC'_{MP}$ is the scaled *EAOC* of the modular plant. R_{max} is limited by lower and upper bounds corresponding to the range of 20% - 90%. The range of α of 0.1–0.9 is selected to model a reasonable experience curve without drastic decreases in cost. The subroutine is solved with the default "trust-region-reflective" algorithm for each point, providing values of R_{max} that bring $EAOC'_{MP}$ the closest to $EAOC'_{con}$. The residual values are only used to select α and R_{max} points that actually provide $EAOC'_{MP} = EAOC'_{con}$. Points with residuals greater than $1 \cdot 10^{-6}$ are discarded.

Figure 15 shows the mapping of learning parameters for the NG price scenarios. When NG is free, the experience curve can behave in a wider range of α and R_{max} values. Whereas when NG is bought at market value, more aggressive learning phenomena should be followed to provide break-even cost.

The required regions of experience parameters are bounded by minimum requirement of experience rate exponent and maximum reduction in price for both price scenarios. The boundaries correspond to curves that suggest tradeoffs between R_{max} and α. A compromise between the two parameters appears towards the left bottom corner, and beyond this region, α and R_{max} grow rapidly. Therefore, balanced and desired learning phenomena are represented by these portions of the limiting curves. Note that break-even is only achieved for combinations of α and R_{max} that fall on the boundary of the illustrated regions. Any point inside the depicted regions provides situations that are better than the break even.

For free NG, less aggressive conditions are related to minimum requirements. An experience rate exponent of around 0.15 and a maximum reduction in price of about 38% are sufficient to achieve break even. For NG at market price, minimum values of about 0.45 and 80%, respectively, are obtained, which corresponds to a much more aggressive learning behavior. If NG price falls in between the analyzed scenarios, the required learning behavior is expected to be bounded by a curve that is also located between the ones associated with each scenario.

Feasible values for both NG price scenarios are chosen to illustrate the outcome of this analysis. Experience rate exponent and maximum price reductions of 0.15 and 40%, respectively, are both greater than the minimum values of 0.15 and 38% for break-even when NG is free. Figure 14 depicts this situation, and as previously stated, modular plants constituted by 90 modular units or more present $EAOC'_{MP}$ that at least break-even with $EAOC'_{con}$.

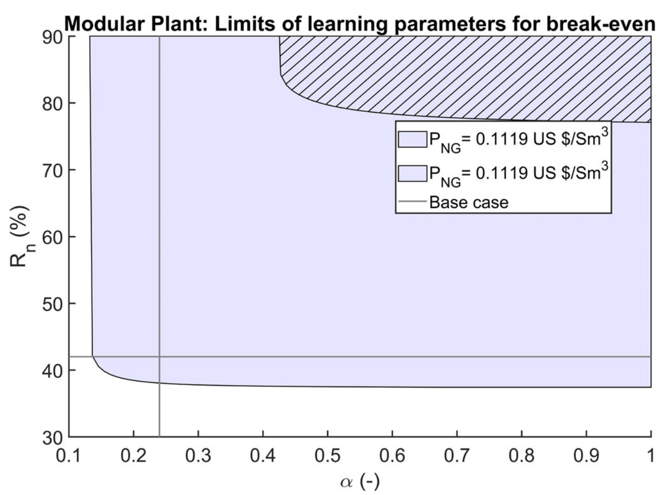

FIGURE 15 Mapping of leaning parameters for NG price scenarios. Base case lines represent values of $\alpha = 0.24$ and $R_{max} = 42\%$, modeled after literature

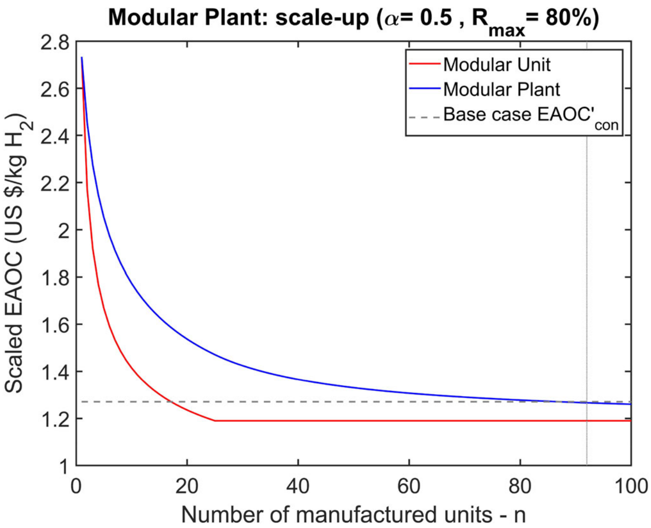

FIGURE 16 Differences between scaled EAOC of a unit and of the plant (cumulative) – $P_{NG} = 0.1119$ US\$/Sm^3. Dotted faded lines correspond to the number of units of 92, required to achieve conventional scale hydrogen production

An experience rate exponent of 0.5, and a price reduction of 80% are values that fit the requirement for break-even cost when NG is at market value. Figure 16 shows the different scaled *EAOC* curves for individual modular units and modular plant in this situation. In comparison with the trend in Figure 14, a steeper and faster decrease in price is required. Technology maturity is achieved at around the 30th manufactured modular unit for the previous case due to a slow experience rate exponent. Here, maturity happens at around 25 modular units, because of a more aggressive experience rate exponent needed to achieve double of the reduction in price.

In general, the bulk purchase of modular units can be used to offset higher purchase costs until technology reaches maturity. A modular plant can be competitively assembled to produce the same amounts of hydrogen as the conventional SMR process when NG prices are closer to zero. When NG is at typical market values, high reductions in price must be present for a longer time, which might not be feasible in practice.

5 | CONCLUSIONS

In this Article, existing TEA methods were extended for costing of intensified modular systems. Adaptations of capital and operating costs were made with a focus on high degrees of process integration and customization. An economy of learning model was incorporated to include the effect of an experience curve into purchase unit price, as modular technology matures.

The developed modular TEA framework included the selection of the parameters that were economically relevant for modular systems deployment. Economic cost indicators were scaled with respect to production of a chemical of interest. Then, a comparative analysis of profitability was performed for small-scale modular capacity. The scaled measures of cost were used to evaluate profitability of individual modular units and of an assembled modular plant. For both cases, competitive scenarios were mapped, showing where the modular process could break even with respect to the conventional counterpart.

A modular hydrogen unit application was developed. An intensified microchannel reactor was considered for this application, and process synthesis around this reactor resulted in a highly integrated modular process. Process operability was used to find feasible operation of the obtained process flowsheet.

The modular TEA framework application to the developed process indicated that the modular hydrogen unit can be profitable in comparison with a conventional SMR plant for scenarios in which NG price is under 0.02 US\$/Sm^3 and the economy of learning produces a reduction of about 40% in purchase cost. The study of contingency and fees showed that the learning phenomenon can also benefit modular deployment when more reliable cost data are provided.

The assembly of a modular SMR plant that consisted of 92 modular hydrogen units was considered for comparison with the conventional industrial scale. Combinations of required experience curve parameters were obtained to achieve break-even cost according to NG price. The economy of learning had to follow less aggressive scenarios when NG is cheap. At NG market prices, reductions in purchase cost needed to be drastic, and therefore, may be unrealistic.

Both individual modular units and modular plant scenarios were significantly favored by low NG prices. This result suggests the modular SMR units are promising in regions with abundant offer of NG, where it is usually flared or reinjected to the reservoir. Remote NG and shale gas formations also present potential for the modular hydrogen units, as conventional SMR plants cannot usually be installed at these locations due to lack of infrastructure.

The presented framework and guidelines provide a platform for studies considering logistics and scheduling. For future studies, the assumption that bulk purchased modular units have the same start-up date could be relaxed. More complex scenarios could be generated, including variable production rates and distinct NG prices at various modular unit locations. As additional reliable data related to modular systems becomes available, cost equations could be updated and thus be made more accurate. Lastly, although logistics and distribution were not the focus of this application, they play a key role as well, especially for gaseous products.[26] Further innovation could be considered in the future to produce new processes that convert natural gas to liquid and solid products such as methanol and carbon nanotubes. This could be explored to facilitate the transportation of hydrogen-derived products. Nevertheless, the developed methodology is based on an ideal scenario, indicating whether the analyzed modular process should be further studied towards manufacturing.

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CONFLICT OF INTEREST

The authors declare no potential conflict of interest.

AUTHOR CONTRIBUTIONS

Vitor Gazzaneo: Conceptualization (equal); formal analysis (lead); methodology (lead); writing – original draft (lead); writing – review and editing (equal). **Madelynn Watson:** Formal analysis (supporting); methodology (supporting). **Carlie B. Ramsayer:** Formal analysis (supporting); methodology (supporting). **Zachary A. Kilwein:** Formal analysis (supporting); methodology (supporting). **Victor Alves:** Formal analysis (supporting); investigation (supporting); writing – review and editing (supporting). **Fernando V. Lima:** Funding acquisition (lead); conceptualization (supporting); formal analysis (supporting); methodology (supporting); writing – review and editing (supporting).

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available from the corresponding author upon reasonable request.

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