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Recognition of Process Safety Position in Multiple-criteria Decision Analysis in Process Design

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Typical factors considered in industrial practice for process designs are material and energy efficiency, process economics and level of environmental burden caused by the new technology. In our work, we propose addition of process safety analysis into the decision-making. To overcome lack of process data known at early design stage, we have utilized safety index methods that are suitable to evaluate process safety level with minimum process knowledge required. Safety indices incorporated into the developed multiple-criteria decision analysis (MCDA) were Process Route Index and Comprehensive Inherent Safety Index. Material and energy efficiency was assessed through E factor and Specific Energy Consumption. Total Capital Cost and Total Production Cost were utilized to assess process economy. Finally, environmental impact was evaluated by C factor and Eco Indicator 99. The proposed MCDA methodology was tested on a case study of hydrogen production from natural gas and biogas. In total, sixteen different process design alternatives were generated and simulated in Aspen Plus. Utilizing Analytical Hierarchy Procedure (AHP) method, different weights were assigned to every calculated criterion to perform MCDA. After assignment of weights, final evaluation matrix for every process design alternative was generated. For easier interpretation of results, viability maps were constructed. Viability map is a 3D figure combining generated case studies, their score in individual criteria and importance of individual criteria represented by its weight. It was found out that natural gas as a feedstock was preferable if considering material and energy efficiency, process economics or process safety as the most important criterion. However, if environmental impact had the highest importance, biogas-based options were the highest rated options. Process safety factor was decisive in specific combination of other criteria. Hydrogen production from natural gas coupled with carbon capture technology for flue gas was identified as the overall best process route.

1. Introduction

The requirements for process design have changed since its origins. Modern sustainable process design necessitates the use of sophisticated analytical techniques. Multiple parameters are supposed to be compared simultaneously and summed up into a single overall predictor that reflects the preference for the process's designed alternative. Several methodologies were already developed for simultaneous evaluation of multiple criteria, grouped by the title of multiple-criteria decision analysis (MCDA), but only a small number of them were applied in chemical process design. In this work, process economics, material and energy efficiency, environmental impact and process safety were considered for hydrogen production assessment (Figure 1).
Selected indicator which characterizes the economics of the process was Total Production Cost (TPC) and Total Capital Cost (TCC). TPC includes the synergy of Total Annual Cost (TAC), TCC, hydrogen product mass flow and selection of desired payback period. TCC was used as a second separate indicator for economics evaluation to assess not only long-term process profitability but also immediate financial demands. Other suitable indicators are Total Operating Cost (TOC) or Total Utility Cost (TUC) to assess energy demands predominantly (Couper et al., 2017).
The material utilization and energy efficiency were evaluated also by two subcriteria. First subcriterion representing material utilization effectiveness was the E factor which is calculated as the ratio of mass of waste

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to mass of product (Woodley, 2020). Energy efficiency was evaluated using Specific Energy Consumption (SEC) as it was employed previously e.g. in the work of Šulgan et al. (2020). SEC is calculated simply as overall energy consumption per mass of product.

Environmental impact is very complex issue that can be assessed by multiple factors, e.g. Global Warming Potential comparing how much of infrared radiation absorbs unit mass of a gas over its atmospheric lifetime to the extent that CO_2 absorbs infrared radiation (Serna et al., 2016), Bio-concentration Factor that represents net result of absorption, transformation and elimination of a substance in an organism due to waterborne exposure (Serna et al., 2016), C factor evaluating how much CO_2 equivalents are produced per mass of product (Woodley, 2020) or EcoIndicator 99 (EI99) that differs from other indicators in its scope and complexity incorporating effects of direct emissions, process equipment manufacture, land usage, etc. (Goedkoop and Spriensma, 2001). In our work, C factor and EI99 were implemented.

Lastly, process safety as a novel addition was assessed. To identify hazard potential, several approaches can be utilized. Due to the usually scarce operating data during early design stage, safety indices are suitable for safety assessment (Roy et al., 2016) in our proposed methodology. Rosa (2020) and Vincent (2020) have analyzed suitability of several safety indices for incorporation into MCDA in chemical industry. In the presented paper, Process Route Index (PRI) and Comprehensive Inherent Safety Index (CISI) were chosen. PRI provides less detailed overview of inherent safety level of different process routes, but it requires less input data (Leong and Shariff, 2009). CISI is more complex safety index to evaluate inherent safety but more thorough process knowledge as input data is required (Gangadharan et al., 2013).

To test the developed methodology, case study of hydrogen production was chosen as a representative process of chemical industry utilizing variety of unit operations, handling typical chemicals and requiring different types of utilities (process water, electricity, cooling water, natural gas, etc.).

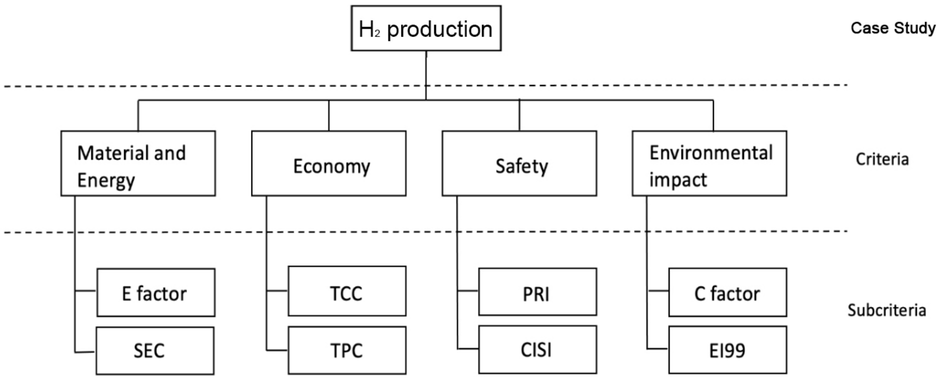

Figure 1: Employed methodology for hydrogen production multiple-criteria evaluation

2. Case Study

Production of hydrogen can be divided into two main categories, based on the source of hydrogen. The first option of hydrogen production, the most applied in industry, is hydrocarbons-based production including catalytic steam reforming, dry methane reforming, partial oxidation and autothermal methane reforming. The other option, energetically more demanding, is water electrolysis. In this work, Aspen Plus simulation of conventional catalytic steam reforming was developed. Generated case studies designed for the proposed MCDA are differentiated by the source of methane. The first, natural gas-based, is the most popular and conventional method for producing hydrogen in industry (labelled NG). The second production alternative is using biogas as a source of methane and is considered a green option (labelled BG).

Multiple process design alternatives were generated. The base case study (Figure 2) consisted of three main units: steam reformer (SR), high temperature water gas shift reactor (HTS) and pressure swing adsorption unit (PSA). Firstly, two sets of steam reforming conditions were generated. First set represented maximum allowable temperature in SR at selected steam to carbon ratio and is labelled “max”. Second set represented variant with decreased temperature in steam reformer by ca. 3 % for better controllability of the process and is labelled “min”. Secondly, additional unit operations were implemented into the base process. These variants included addition of low temperature water gas shift reactor (LTS) (labelled LTS) or carbon capture (CC) (labelled C) technology or combination of both (labelled LTS C). Creating these variants for both, natural gas and biogas feed, generated sixteen different process routes in total. Their overview is summarized in Table 1.

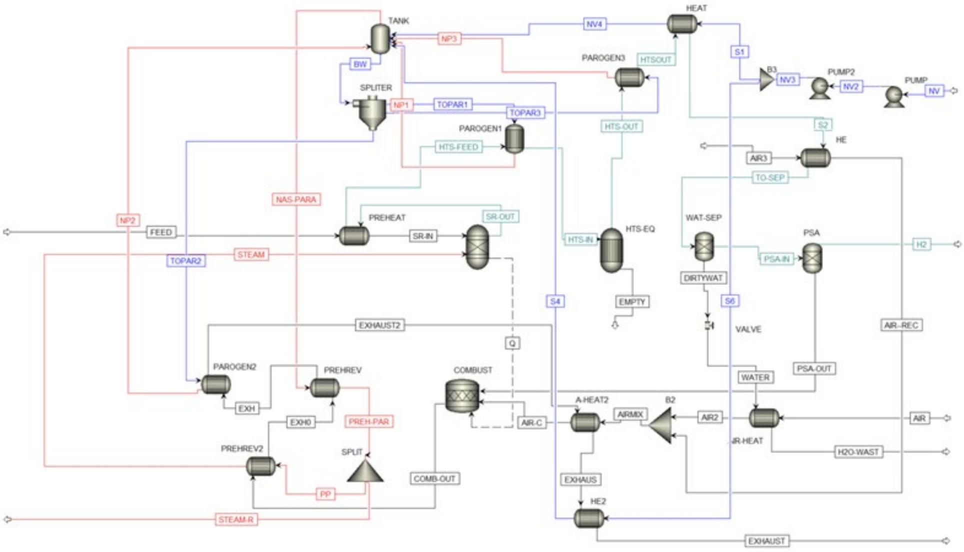

Figure 2: Aspen Plus simulation scheme of base case study of natural gas-based hydrogen production (labelled "NG max" in Table 1)

Table 1: Summary of sixteen generated process routes for the proposed MCDA

No.	Process Route Label	Temperature in SR [°C]	LTS	Carbon capture
1	NG max	850	×	×
2	NG max LTS	850	✓	×
3	NG max C	850	×	✓
4	NG max LTS C	850	✓	✓
5	NG min	825	×	×
6	NG min LTS	825	✓	×
7	NG min C	825	×	✓
8	NG min LTS C	825	✓	✓
9	BG max	720	×	×
10	BG max LTS	720	✓	×
11	BG max C	720	×	✓
12	BG max LTS C	720	✓	✓
13	BG min	700	×	×
14	BG min LTS	700	✓	×
15	BG min C	700	×	✓
16	BG min LTS C	700	✓	✓

3. Results and Discussion

Every generated process route was assessed via aforementioned criteria, i.e. its TCC, TPC, E factor, SEC, C factor, EI99, PRI and CISI values were calculated based on the obtained simulation data. In-depth look at simulation results and calculation of individual criteria can be found in the work of Boháčiková (2021). Example of final values is depicted in Figure 3 for inherent process safety assessed by CISI method. It is noticeable that alternatives with CC technology scored worse using CISI methodology. Large amounts of MEA in process of absorption resulted in much higher hazard potential of the absorption unit and thus overall CISI of process route. This results supports previous findings (Rosa, 2020) that CISI tends to overestimate hazard potential when processing large quantities of material.

After calculation of every subcriteria, final main criterion score (Figure 1) for Material and Energy Efficiency (ME), Process Economics (E), Process Safety (S) and Environmental Impact (EN) was determined. Because of the similar robustness of both subcriteria, only E factor and SEC were assigned the same importance. TPC, CISI and EI99 were assigned two times higher importance, being more robust indicators than TCC, PRI and C factor. In the next step, process routes were ranked according to values calculated for each subcriteria. The ranking was then converted to relative values on scale from zero (worst scenario) to one (best scenario) by dividing each assigned rank number by sum of process routes. For example, the best process route identified by CISI (Figure 3) was NG max, thus gaining one point (16/16). On the other hand, BG min LTS + C was ranked as worst scenario thus its relative score is 0.0625 (1/16).

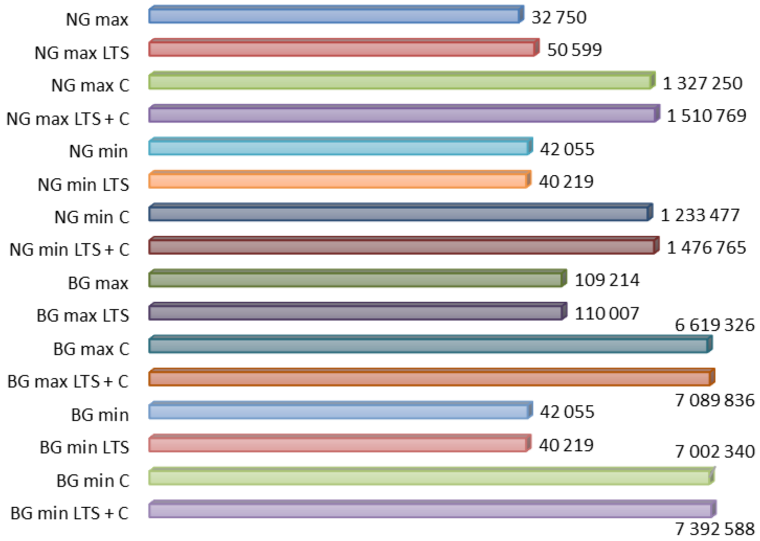

Figure 3: CISI values of all sixteen process routes

The next step was to perform comparisons to build a judgmental matrix. A judgmental matrix was created using integer values constituting a 1-9 scale based on the importance of each main criterion. Different combinations of preferences were generated, e.g. ME being more important than E, E being more important than S and S being more important than EN (ME>E>S>EN) or S being equally important as EN, both criteria being more important than E and E being more important than ME (S=EN>E>ME). Considering all possible permutations, seventy-five different combinations of preferences were created and assessed. In total, sixteen process routes were evaluated by seventy-five possible combinations of preferences and ranked accordingly.

For better understanding of results and their visualization, viability maps (Figures 4-7) were created. Viability map is a 3D figure combining generated process routes, their score in individual main criteria and importance of individual criteria represented by its weight (integer value deciding judgmental value). The colour scale (green – best to red – worst) indicates intuitively the scoring of process routes.

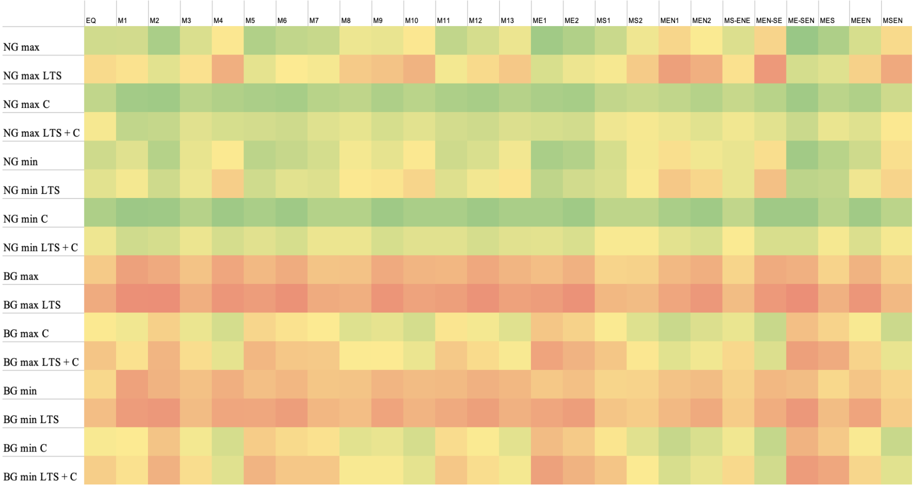

Figure 4: Viability map of scenarios preferring ME and with shared importance including ME (green – best, red – worst)

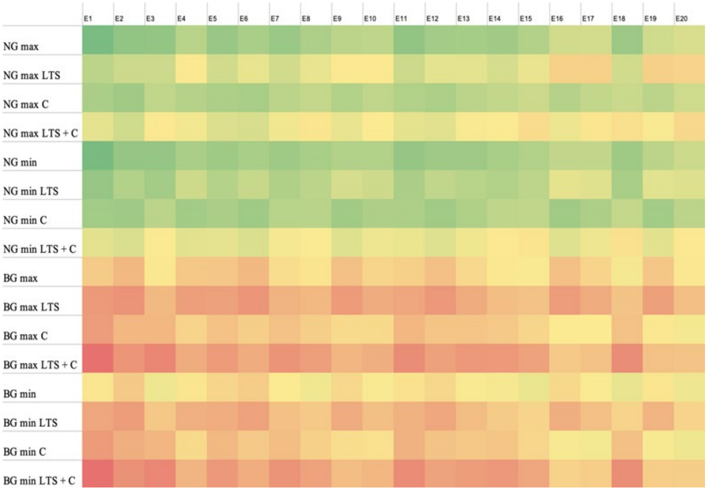

Figure 5: Viability map of scenarios preferring E and with shared importance including E (not present in Figure 4) (green – best, red – worst)

Figure 6: Viability map of scenarios preferring S and with shared importance including S (not present in Figures 4 and 5) (green – best, red – worst)

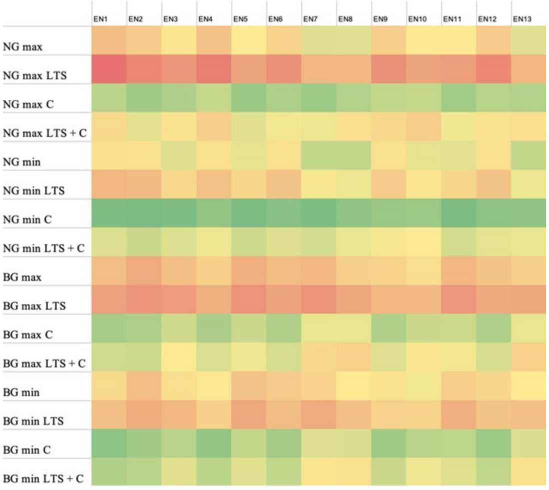

Figure 7: Viability map of scenarios preferring EN (green – best, red – worst)

Figure 4 demonstrated that natural gas as feedstock is more preferable process route of hydrogen production when ME is the most important criterion. Biogas-based process routes (mainly coupled with CC) became competitive for scenarios where E was of the lowest importance. With E being the most dominant factor (Figure 5), biogas-based process routes were always less preferred than natural-gas based ones regardless of the order of other criteria. When S was the most important factor (Figure 6), natural gas-based hydrogen production was not always the highest ranked process route. For scenarios where E was of the lowest importance, biogas-based production coupled with CC (without LTS) was the most preferable design alternative. Figure 7 depicts complete shift in hydrogen production preference toward biogas-based alternative when EN was the decisive criterion.

Analyzing obtained results, NG min C, NG max and BG max C were most often placed in the top three process routes. On the other hand, BG max LTS, BG min LTS, BG max LTS + C were most often placed in the worst three process routes. Generally, biogas-based alternatives were competitive only when process economics was of the lowest importance or environmental impact was of the highest importance. Employing LTS without CC always decreased preferability of the design alternative.

4. Conclusions

Multiple-criteria decision analysis was performed to select the most feasible process route of hydrogen production via catalytic steam reforming. Main criteria for decision making were process economics, material and energy efficiency, environmental impact, and process safety. To provide process data necessary for evaluation, process routes were simulated in Aspen Plus. In total, sixteen different process routes were assessed by seventy-five different decision scenarios with variable preference of each considered criterion.

We found out that addition of carbon capture technology significantly increased the preferability of hydrogen production and using low temperature water gas shift without carbon capture rapidly decreased the preferability of process and sent these cases to the bottom of ranking. Adding process safety and environmental impact shifted feasibility of process routes from natural gas-based production to biogas-based one.

Acknowledgments

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