ABSTRACT: Typically, analysis and design of chemical processes is carried out considering average values of inherently uncertain data that pertain to key design and process variables that shape its performance. In this work, a methodology that includes uncertainty in process safety, an item commonly addressed after the final design has been achieved, along with environmental and economic metrics of the process at the design stage is presented. The approach is based on the use of Monte Carlo simulation techniques to explicitly include uncertainty in the input variables and propagate it through the model. The proposed approach generates a range of performance outcomes through distribution profiles that can be probabilistically characterized, and zones of downside risks and upside opportunities can be identified. A case study that shows the application of the proposed methodology based on the production of ethylene from natural gas was conducted. The results show that although the safest design presented a lower return on investment (ROI), the probability of this scenario to materialize was relatively low, suggesting that a more desirable ROI value for that design would be likely.

1. INTRODUCTION

A typical process design project consists of several stages, namely research and development, conceptual design, analysis, optimization, and detailed design. Typically, once the production route has been selected and the conceptual process design is performed, the process is analyzed to evaluate the overall performance profile of the specific design.1,2 These types of evaluations are usually based on technical and economic analyses, which set the basis for a comprehensive decision-making process regarding the selection or implementation of a certain technology option. Within this common design approach, other aspects such as safety analysis and sustainability properties are considered after the selection of a technology option is made and the detailed design has been completed. In particular, safety assessment of the process leads to the implementation of control loops, barriers, and protection layers as an effort to prevent potentially concerning incidents, as well as reduce the severity of possible outcomes/consequences.3

An alternative approach is to include safety and sustainability components as part of the design of the process. Safety considerations can be implemented through the application of
inherent safety principles. The concept of inherent safety was introduced to establish principles aiming to enhance process safety by eliminating, avoiding, or minimizing sources of risk at the design stage. Indeed, inherent safety principles are better applied at early design stages, given the inherent flexibility to make changes to the process design for the inclusion or further enhancement of key safety characteristics.\(^ {5,5}\)

Even though chemical processes are usually designed to meet specific economic objectives, recent research efforts have also focused on the concurrent development of sustainable and inherently safer process designs. The inclusion of safety concepts in the design stage of chemical processes can be achieved using different techniques. One such technique is the use of quantitative risk analysis (QRA), which represents a systematic and insightful risk quantification approach that includes a comprehensive failure frequency analysis and a consequence analysis in a unified manner. This approach has been creatively followed to design inherently safer chemical systems. In particular, some of the applications of QRA include the design of conventional, multifluect and extractive distillation systems, optimization formulations to select between different production schemes, and the synthesis of intensified designs to guarantee safety and operability performance of a process.\(^ {10}\)

Although QRA provides a useful method to identify inherently safer designs, because of its detailed nature its application is more suited for process systems with only a few pieces of equipment. To evaluate more complex processes, several safety indices have been developed. Such safety indices were introduced in several applications where the relevant input information needed depends on the specific safety enhancement requirements captured by the index under consideration.\(^ {11}\) One of the first indices reported in the literature, with a wide range of applications in the process industries, is the Dow’s fire and explosion index (F&EI). This index is based on material and process factors,\(^ {12}\) and although it requires detailed information about the process under consideration, some simplified versions have been used to assess safety characteristics at the conceptual design stage.\(^ {13}\)

In the Dow’s F&EI structure, the material factor is independent of operating conditions, which has motivated the development of other indices to overcome such a limitation. One of such indices is the Fire and Explosion Damage Index (FEDI)\(^ {16}\) which classifies the units in a chemical process according to potentially hazardous operating conditions. Among its applications, FEDI has been used for the selection of process alternatives to produce ethylene while simultaneously considering safety and economic factors\(^ {17}\) and for the inherent safety assessment of intensified chemical processes.\(^ {18}\) Additional inherent safety indices have been introduced such as the process route index (PRI) and the process stream index (PSI) whose insightful implementation with the aid of an appropriate process simulation software has been persuasively demonstrated.\(^ {19,20}\) These two indices consider stream parameters such as combustibility, energy, density, and pressure to rank processes and streams according to the risk in terms of fire and explosions. The PRI index serves to compare the relative inherent safety characteristics among different processes, while the PSI index provides the relative risk posed by the different streams involved in a given process. Recently, a combination of both indices was used by Ortiz-Espinoza et al.\(^ {21}\) for the multiobjective assessment of different technologies to produce ethylene and methanol accounting for safety, sustainability and economic factors.

Regarding the evaluation of the sustainability performance of a process, techniques to measure the environmental impact of a given design have been developed. Specifically, indicators such as water footprint, greenhouse gas emissions, total waste rate, or more specialized indicators such as the eco-indicator 99 have been used to assess the environmental performance of different process designs.\(^ {8,22,23}\)

Even though substantial progress has been made through the inclusion of sustainability and safety metrics as part of the design of a chemical process, it should be recognized that these evaluations are typically based on performance assessment models that even when they rely on inherently uncertain (random) input variables, only average values are used within the traditional context of the aforementioned approaches, thus overlooking various irreducible sources of uncertainty. This practice therefore may lead to erroneous conclusions regarding the overall process performance profile since it frequently hinges on what is known as the flaw of averages, which states that when process performance is evaluated at average values to represent uncertain inputs in the underlying assessment model, the outcome does not necessarily represent average process performance in the presence of uncertainty (a direct consequence of Jensen’s inequality in probability theory). The problem then is to formulate the model so that a measure of uncertainty in key design variables is included. An effective way to address this challenge is the use of Monte Carlo (MC) simulation methods.\(^ {24}\) MC is one of the most common and accurate stochastic approaches that is conveniently used when problems are highly complex and hard to comprehend and address. The MC simulation method was adopted in this study to (1) enable the explicit incorporation of the uncertainty in input variables of the process model and the direct evaluation of the process performance consequences in the early design phase, (2) simultaneously include the various sources of uncertainty into the model, taking into account the overall effect from possible interactions between them (often conflicting with respect to safety, environmental and economic objectives), as well as the impact of variations in individual variable values, (3) be able to observe the whole range of plant-wide performance outcomes through the distribution profiles of performance indicators, and (4) enable the uncertainty to propagate through the process performance model. Within such a framework, multiple uncertain inputs follow appropriately selected probability distributions, and their respective uncertainty is propagated through the underlying process performance model. As a result, distribution profiles (rather than single-point estimates) for all the key performance metrics are derived that can be statistically characterized. In this manner, ranges of performance outcomes are generated and zones of risks and opportunities are identified. As a result, such an approach provides potentially more valuable insights that can be used by process decision-makers to make more informed decisions when selecting among different design options. Recently, Monte Carlo methods have been used in a similar context to perform economic assessment under uncertainty of different designs involving membrane reactor modules.\(^ {25−27}\) Kazi et al.\(^ {28}\) explored the effects of uncertainty in industrial systems with routine and nonroutine flaring during abnormal situation management. This complex system exhibits rare and sudden transitions that occur over short time intervals. The uncertain nature of flaring incidents was captured within a multiobjective optimization and MC simulation framework for assessing flare mitigation alternatives. Zubo et al.\(^ {29}\) reviewed uncertainty modeling.
methods for modeling uncertain parameters related to complex electricity distribution networks. Within a different context, Kazantzí et al. presented a systematic solvent selection approach in a safety-constrained process system using MC to evaluate system’s performance in the presence of economic and regulatory uncertainties. Other complex systems that have been recently analyzed with MC techniques include those in areas such as project portfolio management, finance and accounting, reliability engineering, operational risk evaluation, value of information studies, and business plans evaluation. A comprehensive review of simulation modeling with various applications was presented in the work of Law (2014).

In the present research work, a systematic integrated framework to explicitly include uncertainty into the performance evaluation stage of chemical process design is developed. In particular, the inclusion of uncertain inputs does not only pertain to the process techno-economic performance evaluation model, but it becomes explicit in the concomitant safety and environmental performance assessment. It should be pointed out that the addition of the safety component to the uncertainty analysis represents a potential advantage for decision-makers, since possible underestimation of process risks in the presence of uncertainty could pose significant challenges.

The rest of the paper is organized in the following way: Section 2 gives a description of the methodology as well as the economic, sustainability and inherent safety metrics used as part of the analysis framework. Section 3 encompasses pertinent results in an illustrative case study whereby the proposed framework is applied for a comprehensive performance evaluation of a technology option to produce ethylene from natural gas. Finally, some concluding remarks are provided in section 4.

2. PROPOSED APPROACH AND FRAMEWORK

We consider the problem dealing with a process design to be evaluated in terms of safety, environmental and economic potential, for which evaluative models incorporating appropriately defined performance indicators are built. In order to avoid a potentially misleading performance characterization and erroneous conclusions that may arise from the use of average values associated with inherently uncertain model inputs, uncertainty related to input variables is first quantified through appropriately defined probability distributions, and propagated through the underlying model with the aid of Monte Carlo simulation techniques. As a result, ranges of potential performance outcomes captured by distribution profiles are generated for all key performance metrics/indicators (as opposed to single-point estimates) that can be statistically characterized, and downside risks and upside opportunities can be explicitly identified for a given process design. These profiles provide decision-makers with a better understanding of the overall behavior of the process under consideration, thus leading to a well-informed and more efficient selection procedure of a process design.

2.1. Uncertainty Analysis. As mentioned above, considering average values for inherently uncertain input variables in a process performance assessment model may lead to inaccurate performance characterizations of a chemical process. To concurrently and effectively include multiple sources of irreducible uncertainty into performance evaluation models of chemical processes, a sequential approach based on MC simulation techniques is considered here, as graphically depicted in Figure 1.

First, a design that provides a base-case flowsheet is needed. Process synthesis principles can be used to generate a design that uses available feedstocks to provide specified products, taking into account chemical routes available and production capacity requirements given by the product demand; alternatively, if a flowsheet is available, it can be used as a base-case structure. Rigorous process simulations are then used to validate the design and provide data on items such as mass and energy balances, equipment sizes, and operating conditions. Then, well-aimed models to evaluate metrics that reflect the level of inherent safety, environmental impact, and process profitability are built. These models are created considering external information, such as product prices or raw material costs, as well as process data extracted from rigorous process simulations. Once the evaluation models have been generated, it is necessary to identify the uncertain inputs that must be considered. Such inputs may be external or inherent to the process, such as operating parameters of the equipment. After the uncertain inputs have been identified, appropriate probabilistic distribu-
tions for the uncertain input variables are determined for uncertainty quantification purposes. These distributions aim to represent the behavior of the uncertain parameters, and they are typically derived using historical data, plant operational data, or data extracted from the pertinent body of literature (comprehensive reports developed by reliable sources, expert opinions, etc.)

Once the probabilistic distributions for the input variables are developed, MC simulations are used to sample random values for each input. The random values for inputs related to process parameters are used to run rigorous simulations to obtain data for the models. In this work, the integration between MC simulations and rigorous process simulations was achieved through an interface created to link the MATLAB and Aspen Plus software environments. In this interface, the MC simulations are performed in MATLAB for the sampling of the uncertain variables, after which such uncertain variables are used to complete the Aspen Plus specifications to run comprehensive simulations. The interface reads the results from Aspen Plus, such as mass and energy balances, equipment sizes, stream parameters, and utilities and waste rates, and uses them to feed the multiobjective assessment model to obtain the performance indicators that need to be evaluated. This step was carried out 10,000 times with the aid of the integrated MC simulator to generate sufficient results and allow an insightful and reliable characterization of the derived profiles of all pertinent indicators.

In particular, valuable statistical information such as minimum and maximum values, mean/expected value, standard deviation, and values at risk and opportunity can be explicitly obtained for each indicator. It is worth noting that the above statistical metrics are associated with the risk-profile of the decision-maker (the expected value, value at risk and value of opportunity, for example, conform to the profile of a risk-neutral, risk-adverse, and risk-tolerant decision-maker, respectively), and therefore the proposed approach offers a more insightful and nuanced perspective in the inherently complex and uncertain world of process performance assessment.

It should be noted that this approach can be used to compare different designs from economic, environmental, and safety viewpoints, or in retrofit applications to analyze existing flowsheets and evaluate the effect that possible changes in operating conditions have on those process performance items. In the application shown in this work as a case study, two designs that differ in pressure conditions of a transformation section of the process were considered.

2.2. Evaluation Models. The selection of the proper metrics for the multiobjective assessment of a process performance is key in order to develop a proper evaluative framework. The selected metrics should be insightful while being easy to compute, compare and of course interpret. The specific metrics used in the present work are described next.

2.2.1. Safety Assessment. In this approach, the process route index (PRI)\(^{19}\) was selected as the inherent safety metric. The metric provides a convenient tool to trace the changes in inherent safety generated by changes in operating conditions of a given process. The metric considers stream parameters such as combustibility, energy, density, and pressure to rank the process design according to its inherent safety characteristics. The information about the stream parameters is conveniently obtained from Aspen Plus and then it is processed to obtain average values of the four parameters. These values are combined to obtain the PRI metric as shown in eq 1.

\[
PRI = \left( \frac{\text{average mass flowrate}}{\text{heating value}} \right) \frac{\text{average fluid density}}{\text{average pressure}} \frac{\text{average combustibility}}{10^6}
\]

(1)

To compute the combustibility term, temperature and composition parameters are combined with flammability limits according to eqs 2–6.

Combustibility is defined as the difference of the flammability limits of a mixture, which are specific for each substance and depend on temperature and pressure. The effect of temperature on the lower and upper flammability limits is accounted for as shown in eqs 2 and 3.

Flammability limits for each compound are modified using a reference temperature (25 °C) and considering the heat of combustion (\(\Delta H_c\)). Then, to account for the interactions between components in a stream, flammability limits for mixtures are computed as shown in eqs 4 and 5. These equations consider the flammability limits for a given compound (LFL\(_c\) and UFL\(_c\)) and its molar fraction (\(yi\)). Finally, combustibility is estimated using eq 6.

\[
\text{LFL}_{-T} = \text{LFL}_c \left[ 1 - \frac{0.75(T - 25)}{\Delta H_c} \right]
\]

(2)

\[
\text{UFL}_{-T} = \text{UFL}_c \left[ 1 + \frac{0.75(T - 25)}{\Delta H_c} \right]
\]

(3)

\[
\text{LFL}_{\text{mix}} = \frac{1}{\sum_{i=1}^{n} \left( \frac{x}{\text{LFL}_i} \right)}
\]

(4)

\[
\text{UFL}_{\text{mix}} = \frac{1}{\sum_{i=1}^{n} \left( \frac{x}{\text{UFL}_i} \right)}
\]

(5)

\[
\text{combustibility} = \text{UFL}_{\text{mix}} - \text{LFL}_{\text{mix}}
\]

(6)

2.2.2. Environmental Impact. For the assessment of the environmental performance of the process, a model inspired by a cradle-to-gate life cycle analysis was developed in order to estimate the total greenhouse gases (GHG) emissions. This model considers the emissions generated due to raw material acquisition and transportation, processing of raw material, and the chemical production process. GHG emissions are calculated via eq 7.

\[
\text{GHG} = \frac{\text{production process emissions} + \text{raw material acquisition emissions}}{\text{raw material processing emissions} + \text{utilities consumption, outlet streams}}
\]

(7)

2.2.3. Economic Metric. The economic performance of the process is measured using the return on investment (ROI) metric. The ROI considers investment costs, i.e. total capital investment (TCI), annual operating costs (AOC), annualized fixed cost (AFC), and annual incomes (AI) and tax rates (TR). Equation 8 shows how ROI is calculated.

\[
\text{ROI} = \frac{(\text{AI} - \text{AOC} - \text{AFC})(1 - \text{TR}) + \text{AFC}}{\text{TCI}} \times 100
\]

(8)
3. CASE STUDY

To illustrate the usefulness of the proposed framework, a multiobjective assessment of a production process that transforms natural gas into ethylene was considered. Two alternatives were earlier designed in the work by Ortiz-Espinoza et al.\textsuperscript{21} one based on oxidative couple of methane (OCM) and another one on a methanol to olefins (MTO) route. It was found that even when the OCM option might be of interest because of its simple flowsheet, an economic analysis showed that it was not profitable. On the other hand, the MTO design, even when it was not optimized, showed a remarkable potential because of its high profitability. Therefore, the process considered in this work as a case study is based on the methanol to olefins route. In this process, natural gas is turned into syngas using a steam methane reformer operating at 850 °C and 20 bar. The outlet stream containing hydrogen, carbon oxides and water is sent to a purification stage where water and CO₂ are removed and the H₂:CO ratio is adjusted to 2. The stream is then pressurized and fed to a catalytic reactor where methanol is produced at 260 °C. The outflow of the reactor is cooled and crude methanol is separated from unreacted syngas. The unreacted syngas is adjusted and sent back to the catalytic reactor. Then, crude methanol is turned into olefins using a methanol-to-olefins reactor (MTO) operating at 450 °C and 1.5 bar. The outlet stream is quenched and water and CO₂ are removed. Finally, the stream is purified and split into different products using a distillation train. Details on the process simulation can be found in the Supporting Information.

This process is now evaluated in terms of its safety, environmental, and economic performance/potential. Nominal values are first analyzed, followed by the application of the methodology presented in this work to account for uncertainty in key design parameters.

The flowsheet shown in Figure 2 consists of three stages, specifically reforming, methanol synthesis, and olefins production. In the work by Ortiz-Espinoza et al.\textsuperscript{21} the process stream index (PSI) was used to detect that the operating pressure in the methanol synthesis loop was the riskiest section of the process (this section is shown in details in Figure 2). On the other hand, the high pressure used for the methanol reactor enhances the economics of the process. Based on these findings, the multiobjective assessment is conducted in this work for two different scenarios, one generating higher economic performance prospects (Design 1, with methanol reactor operating at 83 bar) and the other one aiming to enhance the safety characteristics of the process (Design 2, with methanol reactor operating at 50 bar). To establish a comparison basis, the results of the nominal values for each one of the indicators related to the two designs considered here were evaluated, with the results reported in Table 1. One can initially observe the underlying trade-offs/conflicts that exist among the performance metrics considered in the present study. Operating the reactor at high pressure provides economic and environmental benefits but operating at low pressure yields a safer process.

To incorporate uncertainty in the evaluation models, relevant input variables affecting safety, environmental and economic performance were selected following probabilistic distributions, as outlined in Table 2. Uncertainty in variables that affect the process economics, namely natural gas and product prices, were chosen. Process parameters associated with the operation of compressors (pressure ratio and compressor efficiency) were selected because of their influence on the safety performance profile of the process. Such variables are also important because the pressure is also related to the yield in the methanol production reactor, thus also affecting the economic and environmental performance of the process. The distributions selected for the cost of the natural gas and product prices were derived directly from market data, while the distributions for the compressor-related variables were adapted from similar distributions reported for isentropic efficiencies and pressure ratios of the compressors used in an integrated reforming combined cycle framework.\textsuperscript{38}

![Flowsheet diagram for an ethylene production process via methanol to olefins.](image)

**Figure 2.** Flowsheet diagram for an ethylene production process via methanol to olefins.

| Table 1. Indicators for the Two Designs Evaluated at Nominal Values\textsuperscript{a} |
|---|---|---|
| metric | 83 bar | 50 bar |
| ROI | 29.55 | 22.87 |
| PRI | 9.47 | 5.81 |
| CO₂ | 46.19 | 60.61 |

\textsuperscript{a}Highlighted values indicate the best results for each metric.

| Table 2. Uncertain Inputs and Probability Distributions\textsuperscript{a} |
|---|---|---|---|
| variable | minimum | most likely | maximum |
| compressor-1 pressure ratio (83 bar) | 3.94 | 4.15 | 4.37 |
| compressor-2 pressure ratio (83 bar) | 1.05 | 1.11 | 1.17 |
| compressor-1 pressure ratio (50 bar) | 2.37 | 2.5 | 2.63 |
| compressor-2 pressure ratio (50 bar) | 1.13 | 1.19 | 1.25 |
| compressor efficiency | 0.72 | 0.77 | 0.82 |
| natural gas price ($/kSCF) | 2 | 3.5 | 6 |
| ethylene price ($/lb) | 0.5 | 0.65 | 0.9 |
| propylene price ($/lb) | 0.6 | 0.75 | 1.0 |

\textsuperscript{a}Distribution types were triangular for all cases.
To account for the environmental impact, evaluation of the GHG emissions was calculated in terms of CO₂ equivalents per ton of ethylene, which was used as a functional unit. The choice of GHG emissions was made since this may be the most important item to analyze for systems based on fossil energy sources. The calculation follows a life cycle analysis procedure in which accounting for natural gas extraction is included, and emissions in the production process due to outlet streams and consumption of heat and electricity complete the estimation. The results of process simulations as well as emission factors were considered to compute the total GHG emission. Adjusting eq 7 to the case study, we obtain the following expression for the calculation of GHG emissions,

\[
GHG = \left( \frac{(NG_{\text{tot}})(EF_1) + (NG_{\text{tot}})(EF_2) + (EC_{\text{tot}})(EF_3)}{\text{tons of ethylene}} \right)
\]

where \(NG_{\text{tot}}\) represents the total natural gas consumption (GJ), \(EC_{\text{tot}}\) is the total electricity consumption (MWh), \(HC_{\text{tot}}\) is the total heating utilities consumption (MMBtu), and \(EF\) values are the emission factors, which are reported in Table 3. The summation term accounts for the emissions of the outlet streams of the production process.

### 3.1. Results

Once the models were built and the probabilistic distributions for the uncertain variables were defined, MC simulations were carried out to generate a sufficient number of data points and derive distributions profiles for the three indicators evaluated here. The MC simulations were run for the two scenarios considering high and low pressure for the methanol reactor operation.

Figures 3–5 show the probability distribution profiles for the safety, environmental, and economic indicators, respectively, when all uncertain input variables are varied simultaneously. Table 4 summarizes the relevant probabilistic characteristics/statistical measures for the three indicators evaluated for the two designs.

Figure 3 shows the two distribution profiles for the safety indicator; a lower value represents a safer process. As can be observed, the design with the process operating at 50 bar represents a better alternative in terms of safety. The dotted lines in Figure 3 represent the values for the indicator within the traditional analysis context, i.e. without considering uncertainty explicitly (see also Table 2); one can notice that for the 50-bar scenario, the probability of occurrence of such a value is 55%, whereas the expected value produced by the proposed approach is 5.79 (Table 4) (it is worth mentioning that the MC simulator is an unbiased estimator of the expected value in a probabilistic sense). Therefore, there is a real possibility of misrepresenting process risk under the traditional approach. A similar situation may be observed in the 83-bar scenario, where the probability of occurrence of the value obtained within the traditional framework in the absence of uncertainty is 57%.

The statistical characterization of the safety results in Table 4 suggests that, given the low standard deviation in both cases, values at risk (P95) and opportunity (P5) do not differ significantly from the mean value. Even though changes in this indicator are not significant in terms of safety levels, the inclusion of uncertainty provides a better understanding of the full range of possible safety performance outcomes as well as the associated profile of the process.

The results from the environmental analysis are also shown in Figure 4. In both scenarios, the environmental evaluation results show very little variance; this implies that the specific uncertain variables do not affect significantly this indicator. Emissions of course are higher in the second scenario, as intuitively expected.

Figure 5 shows the ROI distribution profiles regarding the economic performance of the process. It can be clearly observed that a process operation at a higher pressure would benefit the profitability of the process. As far as the significance of the nominal values reported in Table 2, one can observe that for the 50-bar scenario the probability of occurrence of the ROI value obtained within the traditional framework is 53%, while for the 83-bar design the probability of its corresponding value is 44%.

In contrast to the variability in the environmental metric, the economic results show a significant standard deviation. For the 50-bar design, a risk zone (P5, value of risk) is identified at 20.20% of ROI, and for the 83-bar design, the risk zone is at 21.65%. The reward zones (P95, value of opportunity) were found to be located at 32.58% and 39.66% for the 50-bar and 83-bar designs, respectively.

In light of the results offered by the proposed method, it becomes evident that explicitly acknowledging uncertainty and incorporating it within a process performance assessment framework at the process design stage offers valuable advantages. Such an approach could reliably inform the efforts of decision-makers to assess the overall performance profile in an insightful manner.
and sound manner while being aware of risks and opportunities within realistic ranges of possible outcomes.

3.2. Sensitivity Analysis. To complement the results provided by the application of MC simulations, and in order to identify the input variables that affect the process performance profile more noticeably, a sensitivity analysis was carried out. Specifically, Tornado diagrams were developed and the results are presented in Figures 6 and 7 for designs based on reactor pressures of 83 and 50 bar, respectively. Tornado diagrams graphically illustrate the relative impact on the specific indicator’s profile of variations of the different uncertain model inputs. In particular, the change of the expected value of the specific indicator induced by the variation of each input over its prescribed range (from the lowest to the highest value) is depicted with a bar in the Tornado diagram, under the assumption that all other model inputs remain at their baseline values. Afterward, all bars are sorted from long to short, in order to reliably assess the relative impact of the various uncertain model inputs on performance as captured by the associated indicator. Therefore, the major advantage of using a Tornado diagram in this study is to illustrate which uncertain model inputs have the greatest impact on the expected value of all three performance measures/indicators.

Figure 6 shows the Tornado diagram for the design with a reactor operation pressure of 83 bar. As can be seen, the inputs that mostly affect the outcome in the safety evaluation are the compression ratios for both compressors. These parameters affect directly the performance of the methanol synthesis reactor and the stream parameters involved in the methanol synthesis loop are identified as the “riskiest” part in the MTO process. For the environmental analysis, the major variables that influence process performance are the compressors’ efficiency and the compression ratio in the first compressor. Finally, it is shown that economic performance is mostly affected by prices and costs associated with the products and raw material.

The Tornado diagrams corresponding to the design case of a 50-bar reactor operating pressure are presented in Figure 7. Similar inferences regarding the identification of the most consequential model inputs on the three performance metrics can be observed. Similarly to the 83-bar case, the Tornado diagram shows that the uncertain input variables that affect more noticeably the safety indicator are the pressure ratios of both compressors. For the environmental indicator, the variable that most affects the outcome of the analysis is the pressure ratio of compressor 1, instead of the efficiencies of the compressors identified in the previous case. This may be because of the low operating pressure in the methanol production reactor, which causes a high amount of unreacted syngas that must be purged from the system. In the high-pressure design, where reaction yield is high, GHG emissions are higher because of the higher electricity consumption associated with the compressors’

Table 4. Probabilistic Characterization of Results for the MTO Process with Methanol Synthesis

<table>
<thead>
<tr>
<th>scenario</th>
<th>metric</th>
<th>mean</th>
<th>minimum</th>
<th>maximum</th>
<th>standard deviation</th>
<th>P5</th>
<th>P95</th>
</tr>
</thead>
<tbody>
<tr>
<td>83 bar</td>
<td>PRI</td>
<td>9.41</td>
<td>8.54</td>
<td>10.06</td>
<td>0.26</td>
<td>8.98</td>
<td>9.84</td>
</tr>
<tr>
<td></td>
<td>CO₂</td>
<td>46.19</td>
<td>45.91</td>
<td>46.29</td>
<td>0.03</td>
<td>46.14</td>
<td>46.24</td>
</tr>
<tr>
<td></td>
<td>ROI</td>
<td>30.46</td>
<td>13.38</td>
<td>50.94</td>
<td>5.45</td>
<td>21.66</td>
<td>39.66</td>
</tr>
<tr>
<td>50 bar</td>
<td>PRI</td>
<td>5.79</td>
<td>5.36</td>
<td>6.10</td>
<td>0.13</td>
<td>5.57</td>
<td>6.00</td>
</tr>
<tr>
<td></td>
<td>CO₂</td>
<td>60.62</td>
<td>60.52</td>
<td>60.73</td>
<td>0.03</td>
<td>60.57</td>
<td>60.67</td>
</tr>
<tr>
<td></td>
<td>ROI</td>
<td>23.10</td>
<td>4.43</td>
<td>44.71</td>
<td>5.65</td>
<td>13.98</td>
<td>32.59</td>
</tr>
</tbody>
</table>

Figure 4. Probability distribution for the environmental performance of the MTO process

Figure 5. Probability distribution for the economic performance of the MTO process

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efficiency. It was also found that the uncertain input that has the highest effect on the economic metric is the price of the raw material (natural gas), which differs from the previous case in which the major influence on the results was caused by the selling price of the main product (ethylene).

A final test was conducted to compare the effects of individual uncertain variables on the economic performance of the process. This choice was selected because ROI values were shown to be the most noticeably affected by the effect of uncertainty. Figure 8 shows different probability distributions obtained for the MTO process design at 83 bar. The different probability distributions show different scenarios, two of them considering only one variable as uncertain (natural gas cost or ethylene price), another one considering both natural gas cost and ethylene price as uncertain variables, and the scenario where all variables in Table 2 are considered uncertain. As can be observed, natural gas cost and ethylene price have an important influence on the output of the economic model. The natural-gas-only profile shows a

Figure 6. Tornado diagrams for safety, environmental, and economic performance indicators of the MTO process (83 bar).

Figure 7. Tornado diagrams for safety, environmental, and economic performance indicators of the MTO process (50 bar)
similar trend to the one where all variables are considered uncertain in the downside region of the profile, with P5 and P95 values of 22.32 and 33.44 respectively (compared to 21.65 and 39.66 for the case in which all variables are considered uncertain). On the other hand, the ethylene-only profile shows a similar trend to the all-variables profile distribution in the upper part of the profile; calculated P5 and P95 values were 25.41 and 37.58. As expected, considering both variables simultaneously as uncertain produces a more similar result to the case when all variables are uncertain, as confirmed by the P5 and P95 values for this profile that resulted in 21.61 and 38.10, respectively. This supports the information observed in the Tornado diagram where ethylene and natural gas prices emerged as the most influential variables in the economic results.

The sensitivity analysis has complemented the results generated with the use of MC techniques. General and useful remarks on the use of sensitivity analysis can be found in the works by Saltelli et al.32,43

4. CONCLUSIONS

A new systematic framework for the inclusion of uncertainty in the safety, environmental, and economic performance analysis of a chemical process has been presented. The proposed framework offers clear advantages in comparison with the conventional analysis where average input values to a process performance assessment model are used, and single-point estimates are generated by conveniently ignoring underlying sources of irreducible uncertainty. It was shown that one way to address the aforementioned challenge is the use of Monte Carlo simulation techniques to explicitly include uncertainty in the input variables and propagate it through the process performance model. The proposed approach generates a range of performance outcomes through distribution profiles of key performance indicators instead of single-point estimates. It was shown that the derived profiles can be probabilistically characterized such that zones of downside risks and upside opportunities can be naturally identified. Within the proposed context, the distribution profiles for key safety, environmental, and economic performance indicators for the MTO process to produce ethylene were derived in the presence of multiple uncertainties. It could be observed that while safety and economic indicators were significantly affected by the uncertainty in the inputs, the environmental indicator did not exhibit significant variability. In particular, the results show that critical values of key safety indicators in the traditional analysis may not exhibit a high probability of occurrence and, as a result, the associated risks cannot be efficiently managed. Furthermore, the environmental performance-relevant indicator profiles were found to be quite robust to input uncertainty, while the economic ones exhibited great variability. Another advantage of the analysis including uncertainty emerges when a trade-off between objectives exists (the safety and economic performance objectives in this case) where the availability of probability distribution profiles and a range of performance outcomes may inform the selection procedure of design alternatives in a more insightful, nuanced, and sound manner.

ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.iecr.9b02349.

Process simulations conditions (PDF)

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Notes

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