Process Analysis of Hydrogen Production via Biomass Gasification under Computer-Aided Safety and Environmental Assessments

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ABSTRACT: The growing awareness to advance new ways to transform renewable materials for producing clean fuels, under technical and sustainable viability, is evident. In this regard, hydrogen arises as one of the cleanest and energetic biofuels in the market. This work addresses the modeling and evaluation of a biomass gasification topology employing process simulation along with an environmental and inherent safety analysis. The presented pathway considered two renewable raw materials (cassava and rice waste) based on their vast availability in north Colombia regions. We employed Aspen Plus process simulation software to model the process, setting biomasses (and ash content) as nonconventional solids in the software and inclusion of FORTRAN subroutines for handling solid properties. Otherwise, the environmental evaluation was performed applying the waste reduction algorithm (WAR). At the same time, safety assessment involves a comprehensive approach based on the inherent safety index (ISI) and the process route index (PRI) methods. Data generated from the implementation of rigorous process simulation of biomass gasification allowed us to determine the needed aspect for performing process analysis methodologies. Results revealed that this topology generates a total flow of 3944.51 kg/h with more than 97% vol of H2, from the sustainable use of 19,243 kg/h of cassava waste and 15,000 kg/h of rice straw. From the environmental viewpoint, the process showed moderately to a high overall rate of potential environmental impacts (PEIs), with a higher contribution from process sources than energy sources. It indicates that most of the generated impacts would come from self-operation than from the energy supply generation. In the case of process safety, the topology obtained an ISI score of 35, which represents that modeled gasification would operate below 50% of the expected neutral standard for a physical−chemical process. Complementing the safety evaluation, the obtained PRI suggests that compared to other processes, the analyzed topology shows relatively adequate performance considering the nature of this type of process.

1. INTRODUCTION

Nowadays, it is evident that the growing interest of researchers, research centers, and governments for implementing strategies to preserve natural resources has rapidly increased. The application of sustainable development principles has recently attracted much attention in several industries and chemical process facilities.1 There are concerns about the final disposal of solid residues, intensification of energy demand and generation, and rises in the emission of greenhouse gas (GHG).2 As a consequence, the generation of atmospheric pollutants has augmented, as long as fossil fuels remain as the primary energy sources in power generation for the supply of several sectors.3 These correlated facts put pressure on the energy generation sector to create novel ways to mitigate both the effects on the environment and accomplished with the energy requirements demanded by the contemporary society.4 Therefore, production and energy generation from biofuels have appeared, some decades ago, as a realizable alternative to trading-off between pollution prevention actions and summons of economic aspects related to the traditional transformation processes and energy sector.5 Biofuels have the ability to decrease the dependence of fossil fuels, reaching a reduction in GHG emission and carbon footprint; thus, many researchers are optimistic about the potential derived from these substances with a positive prediction regarding biofuels.6 Both identification and designation of suitable feedstock and processing units are among some of the critical aspects to produce biofuels, taking into account the goal of generating them through ecological, economical, and safe operations.7

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In this sense, hydrogen has emerged as a promising fuel platform as long as this compound will perform a role as clean, environmentally friendly, and high-energy content fuel, which is usable in fuel cells to generate electricity. There is a drawback in the commercial distribution of H₂ associated with high production costs; therefore, there is a need to develop strategies and technologies that could make the production of this fuel more sustainable. The use of lignocellulosic material (like crop residues) in transformation processes for the production of hydrogen can both decrease expenses and increase the environmental performance, diminishing potential impacts linked with other types of processing. Colombia possesses a vast potential for the production of bioenergy from residual material, counting the annual generation rates of residues derived from agricultural products such as corn, rice, or cassava. Biomass gasification is a suitable way of producing hydrogen. This technique involves a thermochemical operation under low-pressure and high-temperature conditions. From this technology, hydrogen is generated along with methane, carbon dioxide, carbon monoxide (this mixture called syngas), and several other gases. If the goal is to maximize the production of hydrogen, the process also needs to include further separation stages for syngas purification, water–gas shift (WGS) reaction for intensifying H₂ concentration, and CO₂ capture technologies. Recent studies have had the interest to examine process engineering aspects on biomass gasification. Ishaq et al. developed a biomass gasification topology based on a multigeneration system combining thermoelectric generation for cleaner applications. Zhang et al. incorporated an autothermal CaO looping in biomass gasification for increasing energy efficiency. A novel hybrid system of biomass gasification incorporated photovoltaic energy, hydrokinetic turbines, and biomass gasifiers, achieving better use of resources and reduction of CO₂ emissions. Wu et al. presented a novel steam-air biomass gasification system that combined cooling, heating, and power generation combined with solar energy. Energy and exergy aspects of biomass gasification were discussed by Ebrahimi and Zibasharhag, presenting a novel configuration that included trigeneration of heat, power, and liquified natural gas. Also, gasification technology has been included as a subprocess for production of methanol from biomass in a three-integrated system.

Emerging transformation technologies might involve the use of the biomass/waste-based material, applying industrial production at large scale and Green Chemistry principles. These are examples of chemical facilities that use renewable resources for generating economic profits, reaching reductions of environmental effects derived from the traditional operation. A known disadvantage of the development of this type of process is the high requirements of substantial quantities of utilities, water supply, steam, and other external resources. Reported contributions on process design and analysis have incorporated the environmental assessment for analyzing and diagnosis chemical processes to obtain a more general perception about sustainability and ecological performance. AlNouss et al. compared steam and oxygen fed biomass gasification counting environmental effects based on CO₂ emissions. Moreno-Sader et al. used the waste reduction algorithm (WAR) to evaluate bio-oil production topologies via pyrolysis for valorizing lignocellulosic and algae biomasses. Technical and environmental analyses were applied to assess industrial hydrogen production routes from residual biomass. Petrescu and Cormos examined environmental issues of six integrated gasification-combined cycle configurations. Besides the WAR method, other studies have applied different environmental impact evaluation tools for assessing chemical processes, these methodologies include the life cycle assessment (LCA), which is one of the most implemented techniques for such purposes. This methodology has been extensively applied for process evaluation. DeRose et al. evaluated conversion processes of lipid algae for producing biofuels under LCA and techno-economic assessments. Leceta et al. studied in detail chitosan film production using the LCA method. Safarian et al. implemented an environmental assessment of a small-scale waste biomass gasification based on the LCA method. Han et al. compared typical and resource-efficient biomass fast pyrolysis systems through process simulation and LCA. Salkuyeh et al. employed LCA and techno-economic analysis for studying fluidized bed-based gasification configurations. The Environmental Impact Minimization (EIM) is another tool available for evaluating chemical processes. Otherwise, other contributions have applied the Tool for Reduction and Assessment of Chemicals and Other Environmental Impacts (TRACI). These methods involve analyzing several environmental impact categories grouped as atmospheric and toxicological impacts for the estimation of derived effects on air, water, and soil systems. Environmental assessment needs the knowledge of process inventory for characterizing the environmental effects, depending on the analyzed ecosystem. Hence, the rigorous process simulation framework can provide the data of the process or a bounded system for implementing these environmental evaluation methodologies. It is worth highlighting that the advantage of WAR is that this method shows the rates of environmental impact or effects based on the potential environmental impact (PEI), indicating the velocity on mass and time basis of emissions of measured effects. Therefore, the authors selected this methodology for evaluating the proposed gasification topology.

The inclusion of safety aspects in the evaluation of chemical processes is a relevant task for designing more reliable facilities. Traditionally, process design used to include the protective measures at end design stages, increasing the operating cost of plants due to the need for preventive maintenance and workforce training. Therefore, the inherent safety approach emerged as an alternative that considers the reduction of risk at early design stages by eliminating or reducing the sources of hazards. Many authors have contributed to the growth of the knowledge regarding methodologies and indicators for assessing risks and hazards under chemical processing. The Dow Fire and Explosion Index is one of the most implemented procedures for seeking risk identification, although indicator-based methods such as the inherent safety index (ISI) or the prototype index of inherent safety (PIIS) has been addressed for such purpose. Rathnayaka et al. highlighted that the use of inherently safer design principles has turned into a decision-making tool based on the sustainable process design approach. Process safety remains an active topic regarding process analysis. In this sense, Kidam et al. presented a discussion about the state-of-art approaches on inherent safety evaluation through integrated indicator methods. There are many contributions addressed in the literature evaluating process safety to design of emerging (and existing) transformation technologies.
Gangadharan et al.\textsuperscript{35} introduced a new step-by-step method for counting the safety performance of chemical processes, modifying the conventional ISI. Song et al.\textsuperscript{36} presented a new approach to evaluating inherent process safety in process design via fuzzy logic programming. Other contributions have implemented safety goals for the synthesis and evaluation of chemical processes, simultaneously including environmental and economic aspects. These parameters enhance the influence of using safety principles for cutting the total capital investment and operating costs. Ortiz-Espinoza et al.\textsuperscript{37} applied the process route index (PRI) and the process steam index (PSI) to evaluate safety issues of ethylene and methanol production topologies. They found methodology outcomes regarding the emission factors and cost data. Recently, the evaluation of the process safety of emerging and green-based technologies has attracted much interest regarding the emission factors and cost data. Ortiz-Espinoza et al.\textsuperscript{37} implemented hazard/risk identification and environmental evaluation methods. Safety aspects were measured under Hazard Identification and Ranking (HIRA). It is worth noting that different process analysis tools have been included in the ongoing study of gasification technologies; these include the examination of environmental burdens (previously described), economic/financial features, or technical/energetic aspects (or combination of these). For example, Chambon et al.\textsuperscript{40} assessed biomass gasification based on mini-grid configurations for productive energy applications of rural areas in India, under economic analysis. Both economic and environmental issues have been studied in the power supply chain through the gasification of residual biomass.\textsuperscript{41} Technoeconomic analysis was employed to evaluate financial aspects of a methanol and electricity generation system based on coal gasification.\textsuperscript{42} Madadian et al.\textsuperscript{43} analyzed wood pellet gasification through implementing an algorithm for the minimization of Gibbs free energy. However, it is palpable that there are missing studies addressing process safety and combustibility aspects regarding gasification topologies. So, this study presented here included those issues through implementation of ISI and PRI methods for a topological pathway for production of hydrogen from lignocellulosic biomass.

The described issues confirm the increasing awareness to apply sustainable design principles for studying emerging transformation processes, even for those that address an ecological way of using renewable resources and clean technology principles. Therefore, environmental impact assessment and safety analysis can provide much information about process behavior and technical data to evaluate and diagnose potential improvement areas for achieving more sustainable and reliable chemical processes. Thus, this study is presenting the evaluation of a gasification topology for the valorization of lignocellulosic materials generated in the north Colombia region for industrial production of hydrogen under the WAR along with the ISI and PRI methods. The criteria considered for the selection of these methodologies relate the advantages and information provided by ISI, PRI, and WAR, as reported in Table 1.

Table 1 indicates the features and useful data from the implementation of WAR, ISI, and PRI methods in the evaluation of existing and emerging technologies. Even though recent contributions have studied technical aspects of biomass gasification technologies, the novelty of this study comes from assessing an emerging technology under a comprehensive framework that involves evaluation of environmental issues, general inherent safety aspects, and the more detailed study of flammability and combustibility of handled substances in the process. The last ones provide quite relevant information because gasification technologies necessarily operate under severe operating conditions (high process temperatures and pressures) and handle very flammable substances. Table 2 summarizes recent contributions addressing the implementation of biomass gasification, indicating the used approach and implemented process analysis tool for evaluation of the technology. These data were included in order to enhance the novelty and research scope presented in this research.

As described, there is an absence of reported investigations that have addressed process safety aspects in the study of biomass gasification, while this study is even going deeper by employing the PRI to examine more specific hazards associated with flammable and explosive substances. The novelty also reckons on the consideration of the described technical aspects as a diagnostic and decision-making tool associated with the development of novel ways to take advantage of renewable resources for producing clean fuels. Besides, much of the previous investigations have addressed the analysis of different topologies based on gasification technologies, in which process modeling\textsuperscript{47} and simulation\textsuperscript{48} have served as a powerful tool for providing a straightforward platform in the analysis of gasification technology. Thus, the study presented here used rigorous process simulation, computer-aided environmental, safety, and combustibility assessments of a promising alternative for transformation of rice and cassava wastes, providing comprehensive insights into the continuous progress of thermochemical transformation processes.

2. RESULTS AND DISCUSSION

2.1. Process Simulation. Figure 1 displays the process diagram of biomass gasification simulation. This process involves five main stages; (i) biomass drying, (ii) gasification...
Table 2. Applied Approaches and Implemented Process Analysis Tools in the Evaluation of Gasi

tication Technologies

| feedstock                          | type of gasiification reactions | simulation approach analysis tool                                      | refs |
|-----------------------------------|---------------------------------|------------------------------------------------------------------------|------|
| rice husk                         | rice husk reaction kinetics      | nonconventional solids exergy and energy integrated with combined cycle | 15   |
| olive pits                        | not described                    | exergy and LCA integrated with combined cycle                          | 44   |
| asphaltene and plastic            | Gibbs equilibrium parametric     | steam/gasiification, syngas cleaning and methanol production          | 46   |
| pine sawdust                      | Gibbs equilibrium/nonconventional solids | Gibbs equilibrium with gasification, syngas capture and storage        | 21   |
| pine wood                         | Gibbs equilibrium/nonconventional solids | steam gasification with CO2 capture and WGS and CO2 capture           | 23   |
| coal                              | ChamCAD, Aspen Plus, and CO integration | environmental and parametric gasification, syngas capture              | 22   |
| food waste, manure, and dried sludge | Gibbs equilibrium/nonconventional solids | environmental and EEP, syngas capture, and combustibility              | 19   |
| cassava and rice wastes           | Gibbs equilibrium/nonconventional solids | environmental, интеграл комбинации, и комбинации                  | 28   |

Note:  
- The main objective of this process is the production of highly concentrated H2; thus, we implemented the WGS reaction system, which is an equilibrium reaction to increase the concentration of this fuel from CO and H2O. The equilibrium is favorable to the products when the system develops at 205°C and 32 bar, so this simulation modeled the reactor as an RSTOIC, taking into account the thermodynamic parameters of the equilibrium reactions at the defined operating conditions. The formation of CO2 in the WGS parameters of the equilibrium reactions at the de

The main objectives of this process are to (i) separate CO2 from the syngas, (ii) improve the concentration of H2, and (iii) reduce the amount of impurities in the syngas. Stream 1 and stream 2 represent the inlet flows of raw materials (cassava and rice wastes). The total processing capacity of this plant is 34,240 kg/h of a mixture of these crops' residues. The feedstock goes to a mixing stage and drying unit to remove water content as long as biomass needs to reach less than 10% of humidity before entering the gasifier unit.

As biomass was simulated as a nonconventional solid, it was needed to use the proximal, ultimate, and sulfate analysis for modeling biomass.54 Therefore, this study simulated the drying operation using an RSTOIC reactor model and external FORTRAN calculation, which gives the control parameter of NC biomass and the outlet water content of the mainstream. Superheated air (200°C and 1 atm) was used to develop material drying. This simulation considered the gasification of dried biomass (under nonconventional setting) using a three-reactor system to model the complex reaction mechanism that involves an initial biomass decomposition in its constituent elements (H2, O2, C, S, and N2), following to a separation of ash/char and volatiles which separately burns (BURN-1) and are further mixed for completing gasification reactions (GASIF-1). The whole gasification stage operates at 750°C and 1 atm.50

This stage produces nonclean syngas, including common constituent gases such as CO, H2, CO2, and CH4, along with impurities and solids, which a cyclone (CYC-1) removes from the main process stream. Stream 16 represents the outlet syngas stream of the gasification stage, with a corresponding syngas flow of 28,526 kg/h (excluding impurities, N2, and O2 mixed in this stream). These results showed a conversion efficiency biomass to syngas of 83%, which is within the expected values for this type of processing.51 Therefore, the following stage is syngas cleaning. The nonpure syngas stream continues to a heat exchange unit for cooling in order to reach 15°C. The stream enters to an injector, which uses water as an absorbent medium to remove CO2 and the other gases dissolved in the mixture. A compressor increases the pressure of the flow to 6 bar, and a separator removes reaming water along with the dissolved CO2 and the other gases (stream 22).52

The main objective of this process is the production of highly concentrated H2 and syngas cleaning, (iv) WGS reaction, and (V) CO2 capture. Stream 1 and stream 2 represent the inlet flows of raw materials (cassava and rice wastes). The total processing capacity of this plant is 34,240 kg/h of a mixture of these crops' residues. The feedstock goes to a mixing stage and drying unit to remove water content as long as biomass needs to reach less than 10% of humidity before entering the gasifier unit.

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of 3944.51 kg/h with more than 97% vol of H₂, with remaining portions corresponding to CO₂ and CO. Table 3 summarizes the main mass flows of the simulated biomass gasification process.

### 2.2. Environmental Performance.

The environmental analysis based on the WAR was implemented for the simulated biomass gasification process for the production of H₂. Process simulation provided the needed data about mass and energy flows, property estimation, and production yield, among others, that let to develop the environmental assessment presented in this work. We selected natural gas as the base energy source, considering the recommendation of previous studies for analogous topologies. Figure 2 displays the obtained PEI rates based on the proposed scenarios on time and mass of product basis. In Figure 2, \( I_{\text{gen}} \) refers to the generation rate, while \( I_{\text{out}} \) is the output rate. The results indicate that almost half of the output rate of PEI of this process are generated through the gasification operation, showing a total generation velocity of 4080 PEI/h for scenarios 1 and 2 and 4834 PEI/h for scenarios 3 and 4. Furthermore, the total outlet rate of environmental impacts for these cases corresponds to 8991 PEI/h, 8992 PEI/h, 9755 PEI/h, and 9756 PEI/h, respectively.

Analyzing in detail the overall performance regarding scenario 1 (without energy neither product) and scenario 2 (with the product), it is evident that the contribution of

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**Table 3. Mass Flows and Operating Conditions of Main Streams in the Biomass Gasification Process**

| variable | stream | 1  | 2  | 16 | 23 | 26 | 29 |
|----------|--------|----|----|----|----|----|----|
| temperature (°C) | 25 | 25 | 450 | 15 | 205 | 450 |
| pressure (atm) | 0.99 | 0.99 | 4.93 | 5.92 | 31.58 | 4.93 |
| mass flow (kg/h) | 19,243 | 15,000 | 84,397 | 19,220 | 30,220 | 3945 |
| biomass (kg/kg) | 1.00 | 1.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| ash (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| H₂O (kg/kg) | 0.00 | 0.00 | 0.14 | 0.00 | 0.03 | 0.00 |
| C (kg/kg) | 0.00 | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 |
| H₁ (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| O₁ (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| S (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| N₂ (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| CO (kg/kg) | 0.00 | 0.00 | 0.21 | 0.92 | 0.06 | 0.00 |
| CO₂ (kg/kg) | 0.00 | 0.00 | 0.09 | 0.00 | 0.83 | 0.32 |
| CH₄ (kg/kg) | 0.00 | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 |
| NO (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NO₂ (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| SO₂ (kg/kg) | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| NH₃ (kg/kg) | 0.00 | 0.00 | 0.02 | 0.00 | 0.00 | 0.00 |

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**Figure 1.** Simulation process flowsheet diagram of biomass gasification.

**Figure 2.** Global environmental impacts of the biomass gasification process.
product stream to the generation of impacts is almost negligible, as long as the difference between these cases is 1 PEI/h, which is a marginal value considering the whole process behavior. This outcome is not surprising, taking into account that syngas rich in hydrogen or highly concentrated H\textsubscript{2} represents among the cleanest fuels in the market.\textsuperscript{58} From kg per product calculation, the presented biomass gasification shows a total outlet rate of PEI of 2.47 for scenario 4 (and scenario 3), which indicates that for each produced kg of H\textsubscript{2}, the process will emit 2.47 PEI. Comparing with the literature, the topology presented in this study showed a lower outlet rate of PEI compared with other gasification routes (direct and indirect) that showed generation rates of 5.00, 30.00, and 135.00 PEI/kg of product that involved pressure swing adsorption, selexol adsorption, a combination of these technologies for product cleaning.\textsuperscript{21} The difference between these results might be associated with the implemented technologies for hydrogen production and cleaning (Syngas, WGS, and CO\textsubscript{2} capture) included in this research. Figure 3 shows the overall process and energy contributions to the PEI rate of gasification.

Figure 3. Comparison of the rate of impacts derived from process and energy contributions.

Results in Figure 3 evidence that the environmental effects derived from the energy source do not represent significant contributions to the global generation of PEI, as long as these just correspond to 0.18 PEI/kg of product, which is 7.30% of the total. The environmental evaluation includes the analysis of toxicologic and atmospheric impact categories. This result is an important finding gained from the implemented analysis because it is expected that the severe thermal conditions of the process and its high utility demand might affect the overall life cycle, showing high rates of environmental impacts derived from the supply-to-process energy generation.\textsuperscript{21} Figure 4 shows the results for the toxicologic categories of the biomass gasification process.

Toxicological impacts of the biomass gasification process showed that for the human toxicity by dermal exposure (HTPE) category, there is a consumption of PEI, showing that the effects associated with substances that enter the system are less than the environmental burdens that leave the process or are discharged to the environment. Otherwise, human toxicity by ingestion (HTPI) and terrestrial toxicity potential (TTP) are the most impacted categories of this process, with rates of 0.56 PEI/kg of product (for both topologies) in all evaluated scenarios. Results of the aquatic toxicity potential (ATP) category showed peak values for generation and output rates of 0.03 PEI/kg, indicating that the process would emit or discharge low concentrations of pollutants and toxic substances in aquatic ecosystems. Figure 5 depicts the rate of PEI for atmospheric categories.

Results of Figure 5 reveal that the most impacted category for this group is acidification potential (AP); this metric associated with the potential acidification of the environment as a consequence of reaction mechanisms between water vapor and emitted gases that form acids (in the atmosphere) and return to ecosystems.\textsuperscript{59} Therefore, this velocity of output potential impacts might indicate that the process generates moderate to high gas emissions to the atmosphere that can later end in soils and water bodies. The corresponding rate of environmental impacts for this category is 0.95 PEI/kg for scenarios 1 and 2 and 1.12 PEI/kg for scenarios 3 and 4. These findings show that the energy generation contribution to the global rate is 0.17 PEI/kg, meaning in an outstanding performance as long as previous studies reported high values of this category connected with the effects emitted by energy sources.\textsuperscript{60} The global warming potential (GWP) category was the second most impacted aspect of this process about atmospheric systems, with an outlet rate of 0.14 PEI/kg for all evaluated scenarios. These results correspond to the number of exhaust gases generated from the gasification mechanism, which forms several substances that includes SO\textsubscript{2}, NO\textsubscript{2}, NO, CO\textsubscript{2}, and CO, among others, which affect this long-term environmental atmospheric category. Finally, obtained environmental performance indicates that this process does not involve depletion on the ozone layer according to the resulted rates of impacts for the ozone depletion potential (ODP) category.
Table 4. Summary of Hazardous Properties of Riskiest Chemical Substances

| component          | flammable gas | LEL ± LEL (v/v %) | EX | TLV (ppm) | ROX | total index |
|--------------------|---------------|-------------------|----|-----------|-----|-------------|
| hydrogen           | flammable gas | 4                 | 71 | 4         | N/T | 0           | 8 |
| carbon dioxide     | N/E           | 0                 | N/E | 00        | 1   | 1           |
| methane            | flammable gas | 4                 | 10 | 1         | 1000| 2           | 7 |
| carbon monoxide    | flammable gas | 4                 | 61.5| 3         | 25  | 3           | 10|

“Data provided by ref 62. ^ Data provided by ref 63. * Data provided by ref 64. # Data provided by ref 65. Nonflammable. * Nonexplosive. # Nontoxic.

2.3. Safety Performance. This study implemented a comprehensive safety analysis for assessing a biomass gasification process through the ISI and the PRI. This approach permits evaluating process safety from inherent prevention principles by the information provided from ISI methodology, and the analysis deepens the implications of the mixing properties and the thermal effect on the risk of explosion in the plant under operation.

2.3.1. ISI Results. The assumption of the worst possible situation lets us to assess unknown or uncontrolled situations that affect the inherent safety of a plant. The abovementioned fact implies to establish associated risks generated under process operation. The first aspect evaluated in the ISI method includes chemical substance aspects measured by the chemical inherent safety (CIS) index. The estimation of main and side reaction sub-indexes corresponds to the evaluation of the exothermic degree of the involved reactions in the process. In this sense, gasification reactions are extremely endothermic; therefore, a large amount of energy supply and high temperature is required to develop the reaction mechanisms.

Otherwise, WSG is an extremely exothermic reaction at the conditions developed showing a heat of formation \( \Delta H_f \) equaling to \(-1498 \text{ J/g}\); the corresponding score for main and side reactions are \( I_{RM} = 4 \) and \( I_{SM} = 0 \).

The unexpected chemical reactions and uncontrolled interactions between the components and equipment are a measure through \( I_{INT} \). The gasification process involves the handling and formation of several gases that can form flammable mixtures with air. Hydrogen, methane, and carbon monoxide, among others are good examples of very flammable gases presented in this system. Therefore, \( I_{INT} \) obtained a score of 3 based on the described conditions. The next aspect evaluated by the chemical inherent safety is the hazardous substance index, which counts flammability, explosivity, and toxicity of handled components according to the reported properties commonly found in safety data sheets. Table 4 summarizes the hazardous properties for the riskiest components identified in the modeled gasification topology.

The hazardous substance sub-index was assigned for this process based on the maximum sum of indicators for flammability, explosivity, and toxicity. Carbon dioxide obtained \( I_{h} = 0 \) and \( I_{sp} = 0 \) because this substance is neither explosive nor flammable. Otherwise, hydrogen, methane, and carbon monoxide are very flammable substances that can form explosive mixtures with air in different volumetric proportions. In this sense, \( H_2 \) and \( CH_4 \) show the highest difference between the upper explosive limit (UEL) and lower explosive limit (LEL) with 71 v/v % for \( H_2 \) and 61.5 v/v % for \( CH_4 \). Regarding the toxicity of substances, carbon monoxide is by far the riskiest substance handled in this process with a threshold limit value (TLV) of 25 ppm. TLV measures the level of exposition that a worker can experience after a working day without adverse effects. It also refers to the highest limit that a person can hold without health effects. Therefore, this parameter profoundly affects safety behavior, occupational health, and societal aspects regarding plant operation.

Summarizing, the overall evaluation of flammability, explosivity, and toxicity showed that carbon monoxide presented the maximum hazardous substance index with a corresponding score of \( I_{h} = 10 \). The last sub-index evaluated in the CIS is the corrosivity sub-index \( I_{corr} \) which takes into consideration the information about the corrosivity of substances and considers the recommendation of the construction material for equipment. For those processes that require more specialized and corrosivity, resistant equipment. Considering the AP for the formation of acid-based substances and gases, the majority of processing units need stainless steel as a base construction material. It corresponds to an \( I_{corr} = 1 \) in the process safety section, and this study gives a more detailed description of process equipment, specifying the construction material for them. The required variables for calculating CIS are already determined, so we implemented eq 10, obtaining a corresponding total chemical inherent safety value of CIS = 18.

The next step for the estimation of inherent safety involves evaluation of the process inherent safety (PIS), which in the first case, counts the inventory sub-index of the process. It measures the capacity of equipment (and the plant) to handle the mass flows based on the hydraulic retention time of 1 h. The modeling of the presented biomass gasification process includes the simulation of several processing units such as reactors, vessels, separators, air heaters, and an injector, among others. From a holistic point of view, this topology handles a total inventory of 281.44 t. This value corresponds to the evaluation of the plant, assuming that all processing units belong to the inside battery limits (ISBL). This consideration is supported by the fact that area and size of equipment of the outside battery limits (OSBL) remain unknown at the conceptual design stage.

Therefore, the inventory of the plant means into a score of \( I_1 = 3 \).

It is widely established that temperature indicates the energy and duty needed to operate a process. The hazard and risks increase as long as the lifetime and safety factors of equipment start becoming weaker under very high- or very low-temperature ranges. Therefore, the temperature sub-index in the evaluation of process safety seeks the maximum operating temperature because of the relation between this parameter and the possible danger for human health and life. In the case of the present problem, the maximum temperature locates at the gasification section with a magnitude of 750 °C and a corresponding sub-index \( I_T = 4 \), which is also the maximum possible score for this category. Analogously, operating pressure gives an idea of the potential energy that can affect equipment, generating leaks in the case of containment loss. The abovementioned fact explains that higher magnitudes of this variable pose stern requirements to construct more durable vessels. Commonly, explosions occur by leaks in vacuum equipment and may form explosive mixtures with air and further explosion accidents. In this case, the method sets this...
sub-index searching the highest operating pressure registered in the process, which in this case locates in the WGS section because this operation requires a pressure of 32 atm. This magnitude traduces a maximum pressure sub-index of $I_P = 2$, taking into account the limits based on the Dow E&F Index.

Equipment safety is a very crucial aspect concerned with process safety performance. In this case, we took the same assumption made for the evaluation of inventory regarding ISBL process equipment. As before mentioned, this topology includes several reactor systems, tanks, storage cylinders, heaters, compressors, separation units, among others, which represent themselves associated hazards regarding plant operation. Table 5 described in detail the relevant aspects and characteristics of the equipment used for modeling the biomass gasification process.

### Table 5. Features of Equipment for the Simulated Biomass Gasification Process

| unit      | type of unit  | temperature ($°$C) | pressure (atm) | required material |
|-----------|---------------|--------------------|----------------|------------------|
| MX-1      | solid mixer   | 28                 | 1.00           | stainless steel  |
| HX-1      | air heater    | 200                | 1.00           | carbon steel     |
| DRY-1     | dryer         | 200                | 1.00           | stainless steel  |
| GASIF-1   | gasifier$^a$  | 750                | 1.00           | refractory lining|
| CYC-1     | cyclone unit  | 750                | 1.00           | refractory lining|
| FIY-1     | injector unit | 62.1               | 1.00           | stainless steel  |
| HX-2      | heat exchanger| 15                 | 1.00           | stainless steel  |
| HX-3      | heat exchanger| 450                | 5.00           | stainless steel  |
| PR-1      | compressor    | 261.16             | 6.00           | stainless steel  |
| SP-1      | separator     | 261.16             | 6.00           | stainless steel  |
| MX-2      | tank          | 30.64              | 6.00           | stainless steel  |
| WGS-1     | reactor       | 205                | 32.42          | stainless steel  |
| PR-2      | pressure changer| 750               | 1.00           | stainless steel  |
| BP-2      | check valve   | 144                | 32.42          | stainless steel  |
| FT-1      | filter/membrane| 450               | 5.00           | stainless steel  |

$^a$This operation simulated by parts in three reactors.

The assigment of equipment safety sub-index ($I_{EQ}$) considers the hazards connected with the riskiest processing units, also the severity of specific operating conditions like pressure and temperature. In this case study, much high-risk equipment is used, meaning, in the generation of potential pressure and temperature. In this case study, much high-risk units, also the severity of specifications, considers the hazards connected with the riskiest processing equipment. As before mentioned, this topology is an ISBL process equipment. As before mentioned, this topology is a global point of view, all needed sub-indexes to evaluate PIS and ISI indicators are already known, so we implemented eqs 11 and 9 for estimating them. Table 6 summarizes the specific sub-indexes obtained by developing the ISI method for the simulated biomass gasification process.

### Table 6. Summary of Obtained Results for Evaluated ISI Sub-indexes of Biomass Gasification

| sub-index | score range | gasification | Condition |
|-----------|-------------|--------------|-----------|
| heat of main reaction | $I_{RM}$ | 0−4 | WGS reactor |
| heat of side reaction | $I_{RS}$ | 0−4 | endothermic side reactions |
| chemical interaction | $I_{INT}$ | 0−4 | 3 | hydrogen as very flammable gas |
| flammability | $I_{FL}$ | 0−4 | CO is the riskiest substance |
| explosivity | $I_{EX}$ | 0−4 | 3 |
| toxicity | $I_{TOX}$ | 0−6 | 3 |
| corrosivity | $I_{COR}$ | 0−2 | 2 | refractory lining construction material |
| CIS | $I_t$ | 0−5 | 3 | total process inventory of 281.44 t |
| process temperature | $I_T$ | 0−4 | 4 | 750 °C for gasification reactor |
| process pressure | $I_P$ | 0−4 | 2 | 32.42 atm for WGS reactor |
| equipment safety | $I_{EQ}$ | 0−4 | 3 | operation of high hazard reactors |
| process safety structure | $I_{ST}$ | 0−5 | 4 | moderate to high-risk process structure |
| PIS | 16 | |
| ISI | 35 | |

The results show a PIS value of 16, and the total ISI equals to 35. This study evaluated the percentage of safety at neutral point (% sfn) to determine how far a process would operate from the reference neutral safety point [for detail see eq 12]. The obtained values for this variable in this process were 45.83%, which indicates that this process at the current configuration will operate with an efficiency performance below 50% of the recommended safety standard.

2.3.2. PRI Results. This study implemented the PRI to assess the simulated biomass gasification process considering reported literature, safety data sheets, and self-settings of the evaluated case study. Besides, process simulation provides data
about pressure, temperature, net energy content value, and molar/mass fractions of components involved in the operation. Particularly, the PRI method comprises the calculation of specific substance properties like combustibility, average fluid density, and explosivity limits evaluated at 25 °C (LEL25 and UEL25). The insights that the PRI procedure generate helps to enhance the safety and sustainability evaluation of the modeled gasification process. Table 7 summarizes flammable fluid compounds involved in the gasification process.

| component | \(\Delta H_f\) (kcal/mol) | LFL25 | UFL25 | reference |
|-----------|-----------------|-------|-------|-----------|
| H\(_2\)   | 68.35           | 3.75  | 75.10 | 75        |
| CO        | 67.70           | 12.50 | 74.00 | 65        |
| CH\(_4\)  | 193.19          | 3.80  | 16.90 | 64        |
| NH\(_3\)  | 91.5            | 13.3  | 32.90 | 75        |

Information provided by Table 7 is needed to estimate the combustibility of mixtures and process streams, which is a crucial parameter in the evaluation of PRI. It is worth mentioning that for the estimation of this variable, we considered fluid substances (either gas or liquid) categorized as a flammable component according to the information provided by reported safety data sheets. In this sense, this study identified very flammable substances like hydrogen, carbon monoxide, methane, and ammonia. Aspen Plus provides the other parameters the need to estimate their average value within the system. Table 8 shows the results of PRI and estimated average magnitudes for its calculation for the modeled biomass gasification process.

The average mass heating value \((\text{MHV})_{\text{avg}}\) obtained for this process corresponds to the weighted magnitude of the net heating value of all substances and streams of the system, showing 11,016.37 kJ/kg. This variable is understood as the amount of heat released from the combustion of a specific component from 25 to 150 °C considering the latent heat of vaporization for contained water. The average combustibility value of mixtures \((\Delta FL_{\text{mix}})_{\text{avg}}\) for this process corresponds to 69.62 % vol, representing a very high quantity which is within the expected value for very flammable substances. Otherwise, the average pressure \((\text{pressure})_{\text{avg}}\) remains under a relative low value (3.09 bar), considering the thermochemical nature of this technology. The last evaluated parameter in the PRI method is the average fluid density \((\text{density})_{\text{avg}}\). This variable indicates a general weighted value for density of fluid substance handles in the process. It means that this evaluation dismisses the density of solid components. It is worth mentioning that for the estimation of this variable, we considered fluid substances (either gas or liquid) categorized as a flammable component according to the information provided by reported safety data sheets.

### 3. CONCLUSIONS

This article modeled a biomass gasification process using computer-aided tools to demonstrate the potential and valorize crop residues highly available in north Colombia. The processing capacity of the plant was set according to the regional availability of these materials, which corresponded to 34,240 kg/h of cassava and rice wastes to produce 3945 kg/h of hydrogen. The simulation of the process was accompanied by the implementation of methodologies for process analysis based on comprehensive environmental and safety assessments. In this sense, the WAR method was implemented to determine the PEIs, while safety assessment included the calculation of ISI and PRI methods. Obtained results indicate that gasification topology showed a mid-range generation of environmental impacts, with a rate of PEI of 0.5, for both HTPI and TTP, which were the most affected categories (toxological) by this process. It means that this process both handles and emits chemical compounds that might have moderately low tolerance in the TLV. In the case of aquatic systems, the TTP obtained by the gasification process was quite small (0.03 PEI/kg of product), indicating that the outlet streams would not present disturbing effects on the environment in the event of an unexpected leak of the process. Therefore, the control of process emissions and discharges might be a vital aspect to be considered during operation.

From the global viewpoint, the biomass gasification presented higher rates of impacts associated with its operation than the contribution of energy generation systems. This fact may indicate that the energy requirements of the simulated technology do not represent concerns from the environmental point of view. Comparing with the literature, the presented design showed lower rates of environmental impacts, confirming that the cleaning technologies included in this topology resulted in being adequate from the environmental perspective. These findings associated with environmental performance are positive outcomes as long as the primary goal of this process is to produce a clean biofuel from renewable resources. Otherwise, safety performance in terms of the ISI method showed that this process had less safe behavior for chemical substance sub-index, showing a higher value for that parameter (score of 19) compared with the PIS performance (score of 16). This fact indicates that there are more concerns connected with hazardous properties of handled substances than the features and settings of the process. Likewise, the hydrogen production from cassava and rice wastes gasification obtained a global ISI score of 35, which represents a 45.83% respect to the expected neutral safety standard. Also, the PRI analysis showed that this process obtained a PRI of 2.01, which indicates that the gasification process remains to be a safer alternative in terms of combustibility and flammability that previously evaluated processes like tertiary butyl alcohol production and ethylene production, among others. Direction
for future work may involve further evaluation of energetic, exergetic, and techno-economic aspects in order to get more comprehensive information about its behavior at industrial scale.

4. METHODOLOGY

This study evaluated a biomass gasification process for the production of H\textsubscript{2}, as a strategy for the valorization of the most produced food residues in the north Colombia region. For this purpose, the authors implemented process simulation along with environmental and risk evaluations. The design of the process involves the application of computer-aided process engineering, using material/enthalpy flows, operating conditions, production rates, and unit efficiencies, among others. This study set the processing capacity of the plant, taking into account the reported annual production rates of some of the most produced agroindustry crops in the Department of Bolivar (Colombia). Technical data about process units and operating conditions were taken from the literature and industrial reports. 

Process modeling and simulation generate the information needed for implementing the analysis of the process under atmospheric, toxicology, substance hazards, and inherent process risk aspects. This methodology allows studying in detail technical aspects seeking process improvement opportunities that allow the design of more reliable and sustainable topologies for the valorization of waste-based biomasses and the production of clean fuel like hydrogen. Following, this study describes in detail the step-by-step procedure implemented in this study.

4.1. Process Description and Simulation. The simulation and modeling of chemical processes include a star-point procedure, initiating with the designation of the task in terms of aimed product(s), the establishment of suitable feedstock, and selection of process pathways that their interconnection between chemical and technological layers allow accomplishing the stipulated goal. Once the topology is already synthesized, the method continues to set the involved chemical substances/components, determination of an accurate thermodynamic model and equation(s) of state, setting processing capacity counting raw material market price and availability and considering demanded or needed input conditions about material balances, energy generation/consumption, operating settings (temperature or/and pressure), engineering kinetics, reaction yields, and stoichiometry, among others.

Authors used Aspen Plus process engineering software to simulate biomass gasification for the production of hydrogen from cassava and rice waste. This computational system has several features, configurations, and other aspects that make this a powerful tool for modeling chemical processes. Considering the complexity of involved reactions in gasification, this study input the biomass as a nonconventional solid based on the proximal and ultimate analyses. Tables 9 and 10 show corresponding proximate and ultimate analyses of cassava and rice wastes. The literature has reported several physical–chemical properties of the majority of handled substances in this process. Aspen Plus has a subroutine that estimates the needed properties (both temperature and nontemperature-dependent), which includes variables like Gibbs energy of formation, heat capacity, critical properties, the heat of combustion, among other parameters. This study selected the Peng–Robinson equation of state with the modified Boston–Mathias model to accurately simulate the nonpolar and real behavior of involved substances.

The following assumptions were made for modeling of the biomass gasification process:

- Operation under steady-state
- Solid carbon is used as char
- Tar formation is not considered
- Biomass was entered as a nonconventional solid
- Ash was entered as a nonconventional solid
- Isothermal gasification
- Volatile reactions follow the minimization of the Gibbs free energy

Table 6 shows the general block diagram of the simulated biomass gasification process. The presented process comprises five major stages for processing the lignocellulosic material to high-concentrated hydrogen. It is assumed that biomass enters the systems already preconditioned with the adequate particle size distribution. From a global viewpoint, the presented gasification topology involves (1) pregasification modeling, (2) gasification modeling, (3) syngas purification, (4) hydrogen maximization, and (5) hydrogen purification. The first stage is the drying unit, in which the process removes excess of water content in the raw material as long as the gasification burns biomass under 10% wt humidity. This study modeled this section first defining the nonconventional biomass content for both feedstock inlet flows through the reported data in Tables 9 and 10.

An RSTOIC reactor converts a portion of moisture into water that exits the system as dried flow. To control the outlet stream of dried biomass and the needed amount of dried water, we introduced an external FORTRAN subroutine. Then, the process continues to the next stage, which is the most crucial section of this process because of the main reactions that happen at this point. This study simulates gasification first using an RYIELD reactor that splits NC biomass into its constituent elements, according to the reported proximate and ultimate analyses. This execution also needs to introduce a second FORTRAN calculator that adjusts the computed dry basis content into a wet basis. After the abovementioned operation, the process models volatile substances separately, assuming that the formation of them follows the minimization of Gibb's free energy (RGIBBS reactor). Char, ash, and carbon content divided after decomposition of biomass are mixed with the products of volatile Gibb's reactions along with superheated air, which is the gasifier agent. Biomass gasification comprises a very complex mechanism that involves the development of several chemical reactions. Equations 1–8 show the main reactions related to this system.
CH\textsubscript{2}O\textsubscript{n}N\textsubscript{m}S\textsubscript{p}(biomass) + O\textsubscript{2} + N\textsubscript{2} → CH\textsubscript{4} + CO + CO\textsubscript{2} + H\textsubscript{2} + H\textsubscript{2} + C + ash + TAR + other gases

(1)

2C + O\textsubscript{2} → 2CO

(2)

C + O\textsubscript{2} → CO\textsubscript{2}

(3)

C + 2H\textsubscript{2} → CH\textsubscript{4}

(4)

CO + H\textsubscript{2}O → CO\textsubscript{2} + H\textsubscript{2}

(5)

CH\textsubscript{4} + H\textsubscript{2}O → CO\textsubscript{2} + H\textsubscript{2}

(6)

C + H\textsubscript{2}O → CO + H\textsubscript{2}

(7)

C + CO\textsubscript{2} → 2CO

(8)

Other gases in eq 1 refers to the formation of not desired products in the gasification process. These associated with reactions based on the transformation of N\textsubscript{2} and S, components that comprise the molecular structure of biomass. Therefore, these mechanisms form side gases like NO\textsubscript{2}, NO, or NH\textsubscript{3}.\textsuperscript{85} Subsequently, a hydrocyclone unit separates gas and solid phases of the gasification outlet stream. The solid phase mainly contains residual carbon, char, and ash. The gas stream continues to a cooling unit to reach 15 °C, for further condensation of significant amounts of water. The syngas cleaning stage also involves the operation of an injector-separation system to remove mainly CO\textsubscript{2} along with the other gases mixed in the main flow in the gas mixture, and this system operates under 6 bar. Once the process accomplishes to purify syngas, the design includes the equilibrium reaction WGS (described in eq 5), allowing to increase the production of H\textsubscript{2} from the interaction between CO and H\textsubscript{2}O. Thermodynamic equilibrium is favorable for product formation, setting 205 °C and 32 atm.\textsuperscript{86} An essential drawback of WGS reaction is the formation of vast amounts of CO\textsubscript{2} in which its higher molecular weight makes its yield higher than the corresponding H\textsubscript{2}. Therefore, the process considers a final purification stage for the capture of carbon dioxide to increase hydrogen purity.

4.2. Waste Reduction Algorithm. The WAR is a procedure introduced by the Environmental Protection Agency (US-EPA), which allows determining environmental impacts for the analysis of production processes.\textsuperscript{86} This tool employs the PEI for estimating the effects of arbitrary discharges or emissions of chemicals in the environment. The algorithm also can quantify the rate of PEI generation (or consumption) for processes, counting energy and product streams contributions.\textsuperscript{87} The WAR estimates the environmental performance of a process by calculating eight impact categories grouped as toxicological and atmospheric categories. The first type of indexes include the HTPI, HTPE, ATP and TTP, and the second type comprises the GWP, ODP, photochemical oxidation potential (PCOP), and AP.\textsuperscript{88} Table 11 summarizes the eight impact categories, indicating their equations and reference parameters. The US-EPA offers in its webpage the WARGUI software, which incorporates the WAR method for performing environmental analysis of chemical processes. The selection of this software for evaluating the presented biomass gasification process obeys to the fact that it is entirely free and is available for download on the web.\textsuperscript{89}

4.3. Inherent Safety Index. This study implements the ISI to evaluate process safety for the presented biomass gasification process. The ISI procedure counts the inherent risks connected with the operating variables of a chemical process, along with flammability, explosivity, and toxicity of handled substances. One of the main features of this method involves safety evaluation at the conceptual design stage, which is not a straightforward task as long as there is an absence of information needed for other methods to evaluate process safety performance. The ISI takes into account the contribution of the CIS and the PIS, and it is estimated by eq 9.\textsuperscript{90}

\[ \text{ISI} = \text{CIS} + \text{PIS} \] 

(9)
The ISI considers chemical factors and properties that could affect the inherent safety of the process through assessing parameters like chemical reactivity, flammability, explosivity, toxicity, and corrosivity, among others. Otherwise, the ISI estimates the inherent risks of process operations considering pressure, temperature, equipment safety, inventory, and secure structure. Equations 10 and 11 show the parameters referring to the inherent chemical safety and process safety indicators, respectively.

\[
\text{CIS} = I_{RMAX} + I_{SMAX} + I_{INTMAX} + \left( I_{FL} + I_{EX} + I_{TOX}\right)_{\text{MAX}} + I_{COR}\max \\
\text{PIS} = I_{i} + I_{e}\max + I_{p}\max + I_{EQ}\max + I_{ST}\max
\]

(10)

(11)

where \(I_{RMAX}\) and \(I_{SMAX}\) are the indexes for the main and side reactions. \(I_{INTMAX}\) is the chemical interaction index, \(I_{FL} + I_{EX} + I_{TOX}\)\max is the total dangerous substance index that represents hazardous substance indicator \(I_{\text{max}}\), and \(I_{COR}\max\) is the corrosivity index. In the case of PIS, \(I_{i}\) is the inventory index, \(I_{e}\max\) and \(I_{p}\max\) are the maximum process temperature and pressure indexes, \(I_{EQ}\max\) is the equipment safety index, and \(I_{ST}\max\) is the secure structure index. The safety assessment presented in this study parts from the evaluation of the worst possible scenario or situation that can happen in a chemical process. Through this approach, it is possible to describe the most risk situations that might occur during process operation.\(^{58}\) As the ISI just gives a score or magnitude that not necessarily provides comparable outcomes regarding a safety proof operation, this study used the percentage of safety operation at a neutral point proposed (% sfn) by Meramo-Hurtado et al.\(^{91}\) described by eq 12 as follows

\[
\% \text{sfn} = 1 - \left( \frac{\text{ISI}_i - \text{ISI}_n}{\text{ISI}_n} \right) 	imes 100%
\]

(12)

\(\text{ISI}_i\) is the score for the ISI of process \(i\), while \(\text{ISI}_n\) is the ISI at a neutral point. The last one corresponds to an ISI = 24, as recommended by Heikkila.\(^{32}\) The % sfn can indicate how far is a process, subprocess, or unit (depending on the boundaries) to operate at or under a neutral safety point. Therefore, for those processes that show an ISI score below 24, consequently obtain a % sfn = 100%, as long as in that hypothetical case, the operation would be beyond the standard neutral safety reference.

4.4. Process Route Index. The PRI considered a fundamental variable that counts the results of an explosion accident. Therefore, it evaluates the distance that can be impacted by an explosion, as shown in eq 13. This index counts the mass released and energy, as follows

\[
R_i = C_i (\eta ME_i)^{1/3}
\]

(13)

\(R_i\) is the maximum distance affected by an explosion, \(C_i\) is a constant, and \(\eta = \eta_{\text{Ma}}\) this parameter refers to efficiency and mechanical factors, \(M\) is the total mass of flammable components (kg), and \(E_i\) is the lower limit of heat combustion (kJ/kg). The PRI needs data about mass and energy data, along with parameters like combustibility and flammability, among others. Therefore, the PRI is addressed as follows in eq 14

\[
PRI = f(\text{density, pressure, energy, combustibility})
\]

(14)

In this case, the method considered a variation on the flammability of substance by changes in operating temperature, as shown eqs 15 and 16.

\[
LFL_i = \frac{LFL_{25}}{\Delta Hc} \left[ 1 + 0.75(t - 25) \right]
\]

(15)

\[
UFL_i = \frac{UFL_{25}}{\Delta Hc} \left[ 1 + 0.75(t - 25) \right]
\]

(16)

\(LFL_i\) and \(UFL_i\) are the lower and upper flammability limits for a particular operating temperature \(t\) while \(LFL_{25}\) and \(UFL_{25}\) are the lower and upper limits at 25 °C. \(\Delta Hc\) is the heat of combustion for the analyzed component.\(^{92}\) As the PRI method considers the contribution of mixture properties, the procedure includes calculation of flammability limits of a mixture based on specific values of this variable and the mole fraction of component \(i\) in the mixture, as follows in eqs 17 and 18.

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

(17)

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

(18)

\(\text{LFL}_{\text{mix}}\) and \(\text{UFL}_{\text{mix}}\) are the corresponding lower and upper flammability limits of an evaluated mixture, \(x_i\) is the mole fraction of component \(i\), LFL\(_i\) and UFL\(_i\) are the defined lower and upper flammability limits of component \(i\). The above-mentioned equations provide the data needed about flammability information, so PRI calculation includes evalu-
tion of average parameters for heating value, fluid density, pressure, and flammability of mixture, as follows in eq 19.

\[
PRI = \frac{(\text{mass heating value})_{\text{avg}}(\text{density})_{\text{avg}}(\text{pressure})_{\text{avg}}(\Delta FL_{\text{mix}})}{\varepsilon_c}
\]

(19)

\(\Delta FL_{\text{mix}}\) is the difference between flammability limits of a mixture, \(\varepsilon_c\) is an empirical constant defined in this case to be equal to 10\(^8\). The process data needed for implementing the PRI method can be obtained from simulations in Aspen Plus.

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