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Assessment of Intrinsic Hazards in an Energy-Integrated Gas Oil Hydrocracking Process

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Abstract

This study assesses the intrinsic hazards of an energy-integrated gas oil hydrocracking process from a sustainability-oriented process safety perspective. Hydrocracking units are essential in modern refineries for upgrading heavy gas oil fractions into higher-value fuels; however, they operate under severe conditions involving high temperatures, elevated pressures, hydrogen-rich environments, complex process structures, and large inventories of hazardous substances. In this context, improving energy efficiency through heat integration must be evaluated together with its implications for inherent safety and sustainable process design. The Inherent Safety Index (ISI) methodology was applied at the conceptual design stage to quantify the intrinsic risk level of the process and identify the main contributors to chemical and process-related hazards. The results yielded a total ISI value of 46, composed of a chemical safety index of 26 and a process safety index of 20, indicating a high intrinsic hazard level. The most significant contributors were toxic exposure (I_{TOX} = 6), inventory magnitude (I_I = 5), and process structure (I_{ST} = 5), while the large ISBL inventory of 2838.3 t, together with operating conditions reaching 456.4 °C and 166.8 bar, substantially increased the inherent risk of the system. Although energy integration contributes to improved thermal performance, the results indicate that it does not significantly reduce the intrinsic hazard level. Sensitivity analysis showed that optimization of operating temperature and pressure could reduce the ISI from 46 to approximately 43. These findings demonstrate that the intrinsic risk of energy-integrated hydrocracking systems is primarily governed by operating severity, hazardous material inventories, and toxicity, highlighting the importance of incorporating inherent safety principles during the conceptual design stage to achieve safer, more resilient, and more sustainable refinery operations.

Keywords: gas oil hydrocracking; intrinsic hazards; energy integration; inherent safety index; sustainable refinery design; process safety

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1. Introduction

The transition toward more sustainable industrial systems requires not only improvements in energy efficiency, resource utilization, and environmental performance but also the systematic reduction in intrinsic hazards embedded in process design. In this context, inherent safety has become an essential principle for chemical and refinery operations, particularly after a series of major industrial accidents that exposed the limitations of relying exclusively on add-on protection systems and operational controls. One of the most

influential events was the Flixborough disaster in 1974, which demonstrated that complex process modifications, large inventories, and insufficient consideration of intrinsic hazards can lead to catastrophic consequences when safety is treated mainly as an external layer of protection [1]. This lesson was reinforced by the Bhopal accident in 1984, widely recognized as one of the most severe disasters in the history of the chemical industry, where the release of methyl isocyanate caused thousands of fatalities and revealed the consequences of storing and handling highly hazardous substances without adequate integration of safety into the process concept itself [2]. In response to these events, Trevor Kletz formalized the philosophy of inherently safer design, emphasizing that hazards should be eliminated or reduced at their source rather than controlled only through safeguards that may fail [3]. His well-known principle, "what you don't have, can't leak" [4], summarizes the logic of minimizing inventories, simplifying process configurations, moderating operating conditions, and substituting hazardous materials whenever possible. From a sustainability perspective, this approach is highly relevant because accident prevention is directly connected with worker protection, community safety, environmental preservation, asset integrity, and long-term operational resilience.

The incorporation of inherent safety criteria during the early stages of process development is especially important because many of the most decisive safety and sustainability outcomes are defined before detailed engineering and plant operation. Decisions related to process configuration, equipment selection, heat recovery networks, operating pressure, temperature, material inventories, and chemical routes determine the intrinsic hazard profile of the facility [5]. Heikkilä et al. emphasize that integrating safety criteria at the research and conceptual design stages provides the greatest opportunity for hazard reduction, since later modifications are usually more limited, expensive, and dependent on additional protective systems [6,7]. This consideration is particularly relevant for gas oil hydrocracking, a key refinery process used to convert heavy hydrocarbon fractions into lighter and more valuable fuels. Although hydrocracking contributes to product upgrading and refinery flexibility, it operates under severe thermodynamic conditions, involves high-pressure hydrogen systems, and handles large inventories of flammable, explosive, toxic, and corrosive substances. These characteristics make hydrocracking units critical from both process safety and sustainability viewpoints. In refinery environments, the absence of inherently safer alternatives or the insufficient consideration of design-related vulnerabilities has contributed to severe accidents, as illustrated by the 2005 Texas City refinery accident, where process design weaknesses combined with operational failures led to the release and ignition of light hydrocarbons, causing multiple fatalities [8,9]. Such events show that sustainable refinery design cannot be limited to energy and material efficiency; it must also address intrinsic risk reduction as a core design objective.

Several quantitative and semi-quantitative tools have been developed to evaluate process safety, with their applicability depending on the level of information available and the stage of project development [10]. Among these tools, the Inherent Safety Index proposed by Heikkilä provides a structured framework for assessing hazards associated with chemical substances, reaction behavior, operating conditions, equipment characteristics, inventory, and process structure during the conceptual design phase [11]. This makes it particularly useful for identifying critical contributors to intrinsic risk before design decisions become fixed. Although the ISI methodology has been applied to different chemical processes, its application to energy-integrated gas oil hydrocracking units remains limited. This gap is relevant because energy integration modifies heat recovery schemes, thermal interactions, process connectivity, and operational complexity. Therefore, even when heat integration improves thermal efficiency and reduces external energy demand, its influence on intrinsic hazards is not necessarily favorable or self-evident. In this sense, evaluating

energy-integrated refinery processes requires a broader sustainability-oriented perspective that considers not only energy savings but also safety implications, accident prevention, environmental protection, and resilience under high-severity operating conditions.

Accordingly, this study assesses the intrinsic hazards of an energy-integrated gas oil hydrocracking process using the Inherent Safety Index at the conceptual design stage. The analysis quantifies the overall inherent safety level of the process, identifies the most critical chemical and process-related subindices, and evaluates whether energy integration contributes to reducing or maintaining intrinsic risk. By focusing on a high-pressure hydrogen-intensive refinery process, this work provides design-oriented insights for safer and more sustainable hydrocracking systems. The results are intended to support early-stage decision-making by showing how sustainability in refinery operations should integrate energy efficiency with inherent hazard reduction, occupational safety, environmental responsibility, and prevention of major accident scenarios.

The remainder of this paper is organized as follows. Section 2 describes the energy-integrated gas oil hydrocracking process and the methodology used for the inherent safety assessment based on the Inherent Safety Index (ISI). Section 3 presents and discusses the results, including the evaluation of chemical and process safety subindices, the overall ISI value, the sensitivity analysis, and the comparison with alternative case studies reported in the literature. Finally, Section 4 summarizes the main findings and provides recommendations for improving the inherent safety performance of hydrocracking systems.

2. Materials and Methods

2.1. Process Description

The gas oil hydrocracking process is composed of six main stages, reaction stage, hydrogen recovery and makeup, stripping, debutanization, naphtha separation, and fractionation; its overall configuration is illustrated in Figure 1 through a block flow diagram that presents the main process streams and unit sections, providing a comprehensive view of the process structure and clearly showing the interconnections among the stages. The equipment identifiers used throughout this study (e.g., reactors, columns, heat exchangers, fired heaters, separators, pumps, and air coolers) correspond to generic process units defined within a process modelling environment and are intended solely for process representation and safety assessment purposes. They do not refer to specific commercial equipment, manufacturers, or proprietary models.

2.1.1. Reaction Stage

The hydrocracking process begins with the mixing of 221,147 kg/h of fresh gas oil (Stream 1) at a temperature of 112.2 °C with 22,515 kg/h of makeup hydrogen (Stream 3) at 118.3 °C. The fresh feed consists of a blended gas oil mixture composed of heavy coker gas oil (HCGO), medium vacuum gas oil (MVGO), and light cycle gas oil (LCGO). The mass composition of the gas oil feed stream and the makeup hydrogen is presented in Table 1.

Table 1. Mass fraction of the fresh feed stream to the hydrocracking unit.

Component	Mass Fraction
Heavy Coker Gas Oil	0.327
Medium Vacuum Gas Oil	0.523
Light Cycle Gas Oil	0.15

The fresh feed stream, combined with makeup hydrogen, is preheated from 116.6 °C to 264.9 °C through a network of heat exchangers that recover thermal energy from hot process streams, thereby enhancing the overall energy efficiency of the system. Subsequently, the

mixture is heated in the fired heater FH-100 to reach 379.4 °C and 165 bar, conditions under which it is fed to reactor HCR-100 together with 34,873 kg/h of hydrogen (Stream 15) at 65.56 °C and 167.8 bar. In this reactor, hydrocracking and hydrogenation reactions occur in the presence of bifunctional catalysts [12], promoting the conversion of heavy hydrocarbons into lighter fractions and stabilizing the intermediate fragments generated during molecular cracking [13]. The typical reactions of the process are summarized in Table 2.

Table 2. Main reactions involved in hydroprocessing units.

Reaction Type	Reaction
Aromatic Hydrogenation	$C_6H_6 + 3H_2 \rightarrow C_6H_{12}$
Hydrocracking of Long-Chain Paraffins	$R - C_5H_{11} + H_2 \rightarrow C_5H_{11} + R$
Hydrocracking of Naphthenes	$C_{10}H_{20} + H_2 \rightarrow C_6H_{12} + CH_4$
Hydrocracking of Polycyclic Aromatics	$C_{14}H_{10} + H_2 \rightarrow C_{10}H_{12} + C_8H_{16}$
Hydrodenitrogenation	$C_5H_5N + 5H_2 \rightarrow C_5H_{12} + NH_3$
Hydrodeoxygenation	$C_6H_6O + H_2 \rightarrow C_6H_6 + H_2O$
Hydrodesulfurization	$C_4H_{10}S + H_2 \rightarrow C_4H_{10} + H_2S$
Olefin Hydrogenation	$C_6H_{12} + H_2 \rightarrow C_6H_{14}$

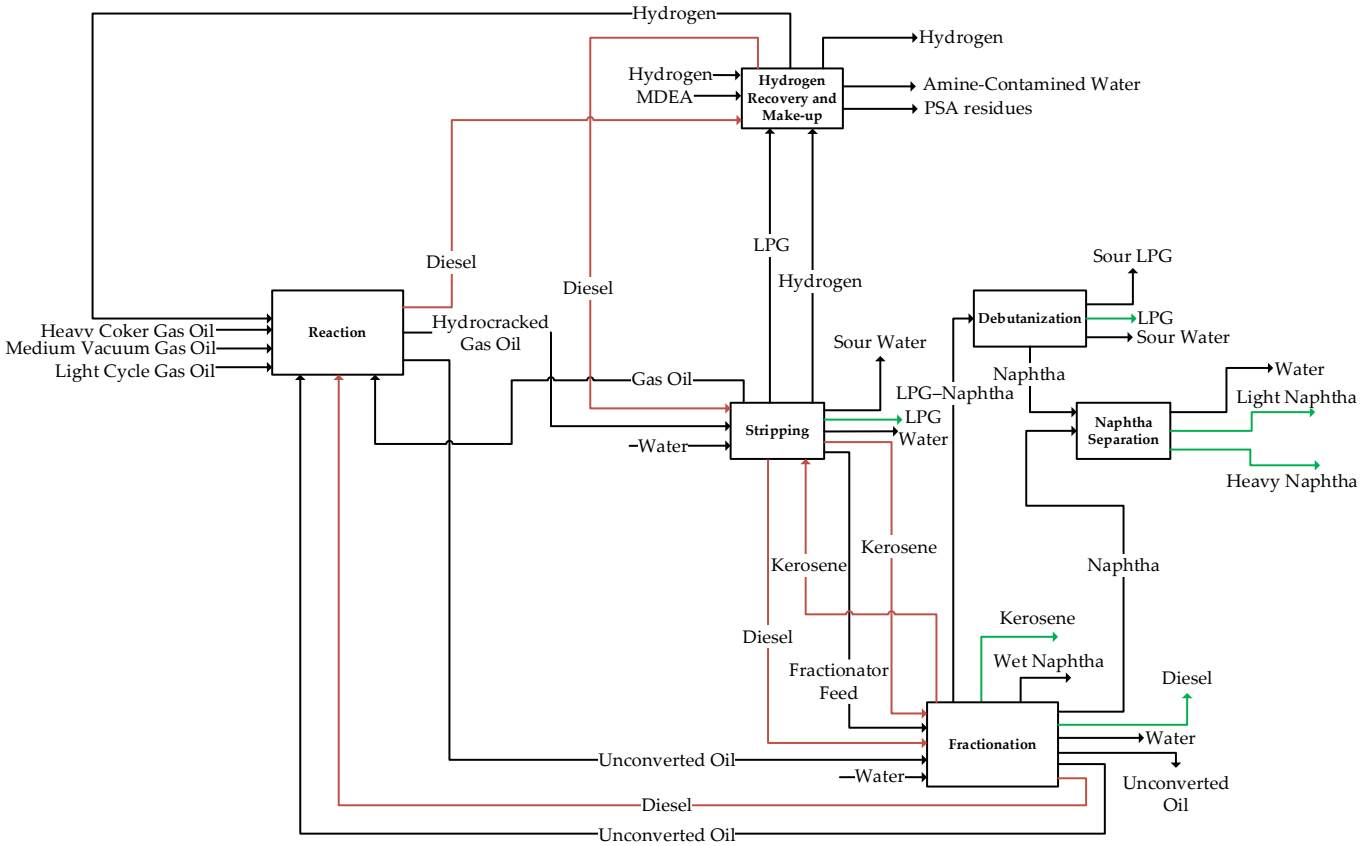

Figure 1. General block flow diagram of the energy-integrated hydrocracking process.

Similarly, hydrocracking reactions also take place in reactor HCR-101; however, in this case, the feed consists of unconverted oil (UCO) from the bottom of the fractionation column T-104, at a flow rate of 185,384 kg/h. This stream is previously cooled in the air cooler AC-107 from 456.3 °C to 382.2 °C (Stream 22). Additionally, 22,645 kg/h of makeup hydrogen at 118.3 °C (Stream 23) and 8574 kg/h of recovery hydrogen at 65.56 °C (Stream 24) are supplied to the reactor. At this stage, hydrocracking of aromatic, naphthenic, and paraffinic compounds is particularly relevant, each contributing differently to conversion severity

and product distribution [14]. Finally, the effluents from reactors HCR-100 and HCR-101 (Streams 29 and 30) are mixed and sent to the stripping stage in the component separator V-100. The process flow diagram of the reaction section is shown in Figure 2.

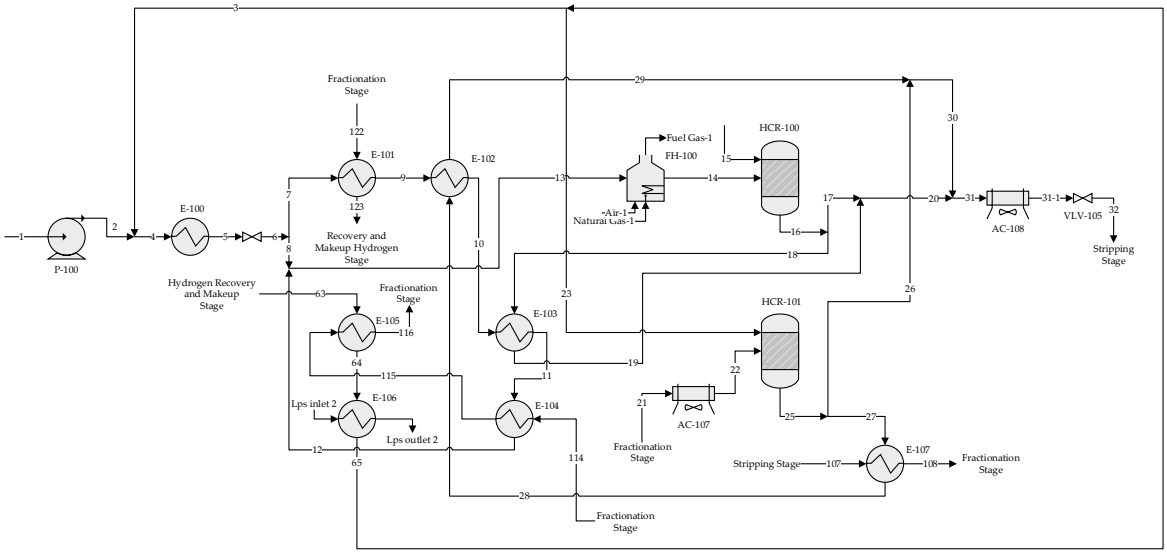

Figure 2. Reaction stage of the energy-integrated gas oil hydrocracking process.

2.1.2. Hydrogen Recovery and Makeup

In the hydrogen recovery and makeup section, 32,628 kg/h of makeup hydrogen is introduced, and a total of 80,528 kg/h of hydrogen (Stream 50) is recovered through the absorption column T-100; part of this recovered stream is mass-integrated into reactors HCR-100 and HCR-101, corresponding to Streams 15 and 24, respectively. Additionally, the makeup hydrogen stream is thermally integrated with hot streams from the bottoms of the distillation columns in order to improve the overall energy efficiency of the process. Specifically, the hydrogen temperature is increased from 103.4 °C to 114.7 °C in heat exchanger E-113, which recovers energy from the bottoms of column T-105; subsequently, the stream is further heated to 116.2 °C in heat exchanger E-105, using the bottoms of column T-104 as the heating medium. This section is shown in Figure 3.

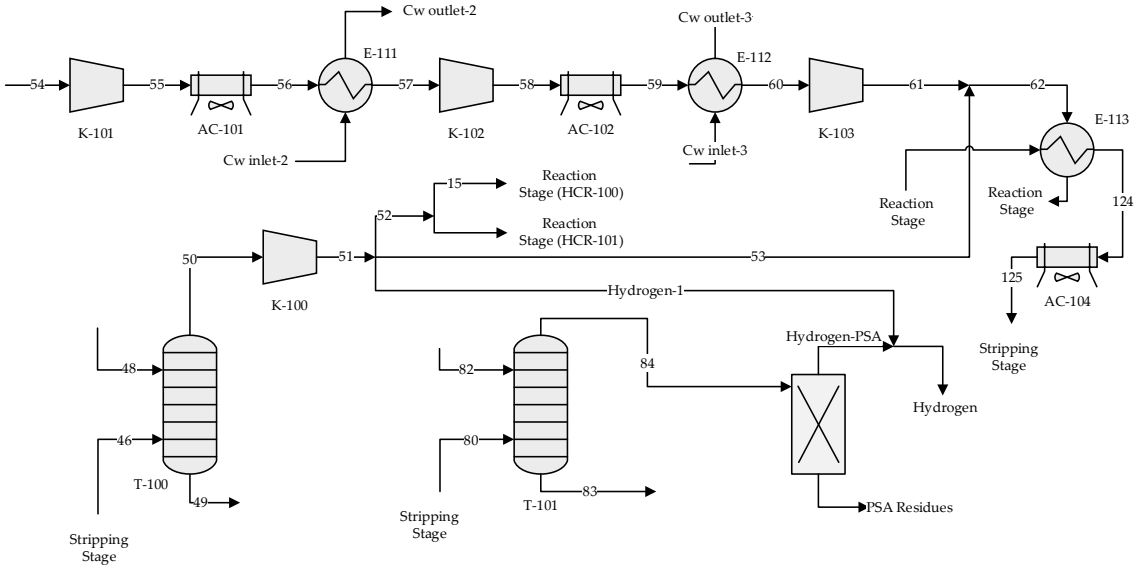

Figure 3. Hydrogen recovery and makeup stage of the energy-integrated gas oil hydrocracking process.

2.1.3. Stripping Stage

The stripping stage includes energy integration between internal process streams and streams from the fractionation section, occurring in heat exchangers E-108, E-115, E-117, and E-119. Although the bottom streams of the three distillation columns in this stage exhibit high temperatures and are integrated with other sections of the process, no additional energy integration is observed strictly within the defined boundaries of the stripping stage. This stage is illustrated in Figure 4.

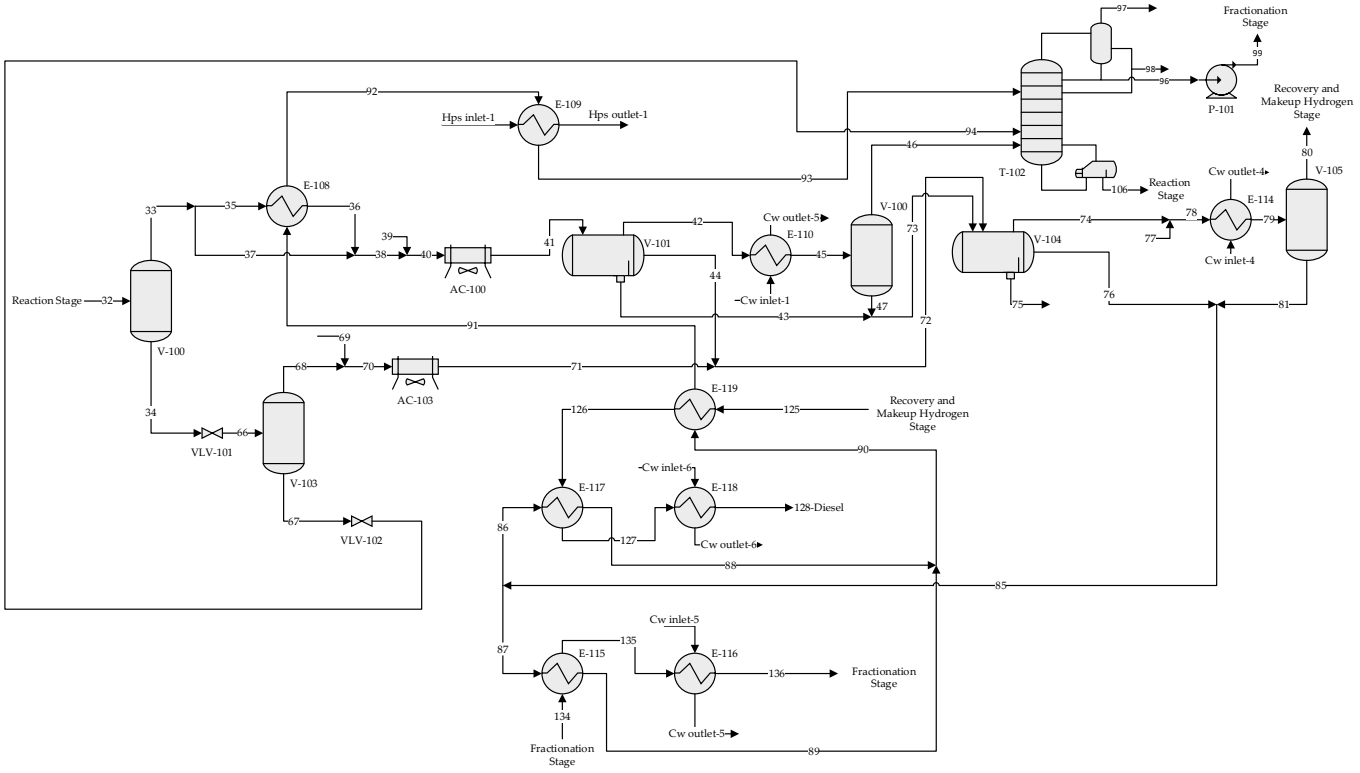

Figure 4. Stripping stage of the energy-integrated gas oil hydrocracking process.

2.1.4. Debutanization Stage

In this stage, 16,651 kg/h of naphtha is fed into the distillation column (T-103) and heated from 88.1 °C to 133.9 °C; during this process, 3772 kg/h of LPG is removed through the overhead stream, while 12,715 kg/h of LPG-free naphtha is recovered from the bottom stream (Stream 144) and sent to the naphtha separation stage for further processing, as illustrated in Figure 5.

2.1.5. Fractionation Stage

The fractionation stage, illustrated in Figure 6, separates the liquid hydrocarbon stream into lighter products and heavier fractions through a series of distillation columns. This stage begins with a feed of 389,806 kg/h from the bottom of column T-102, which contains approximately 16% kerosene, 26.2% diesel, and 50.6% unconverted oil (UCO), with the main objective of maximizing diesel recovery. Prior to entering the fractionation system, the stream is heated in a fired heater (FH-102), raising its temperature from 354.2 °C to 379.4 °C and reaching a pressure of 2.932 bar before being fed into column T-104, where an additional 3889 kg/h of steam is introduced to strip kerosene and diesel from the UCO. As a result, 194,498 kg/h of UCO (Stream 112) is obtained from the bottom, of which 95.3% is recycled to the hydrocracking reactors (HCR-101). The distillate from column T-104 (Stream 111) is then fed at a rate of 199,197 kg/h into column T-105 under conditions of 281.8 °C and 1.358 bar, where 106,587 kg/h of diesel is

recovered as the bottom product (Stream 128—Diesel), while 92,610 kg/h of the distillate (Stream 120) is sent to column T-106 at 190 °C and 1.772 bar, yielding 60,537 kg/h of kerosene from the bottom stream.

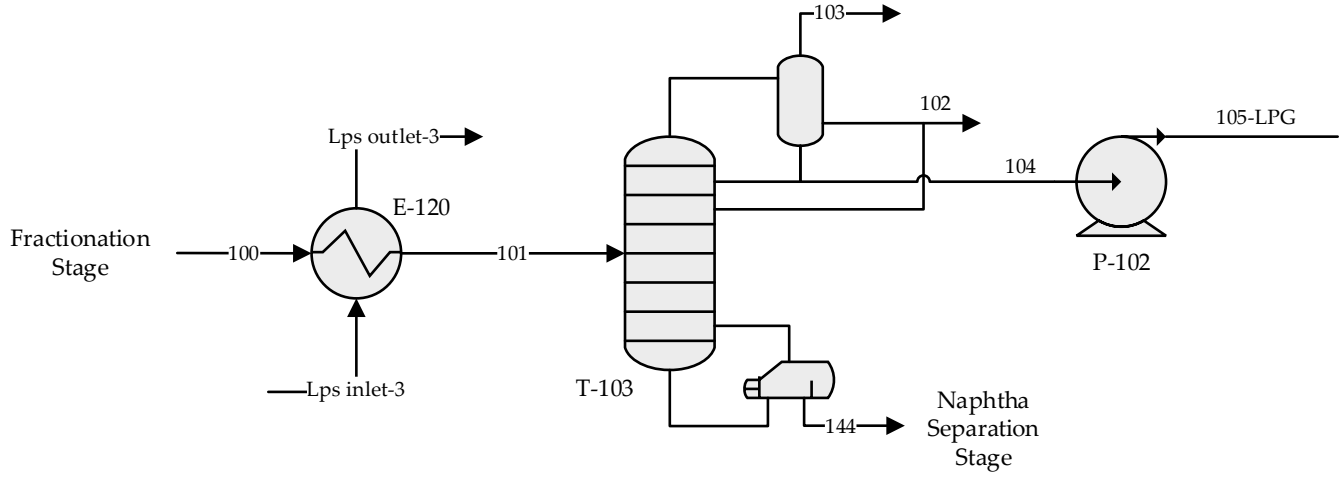

Figure 5. Debutanization stage of the energy-integrated gas oil hydrocracking process.

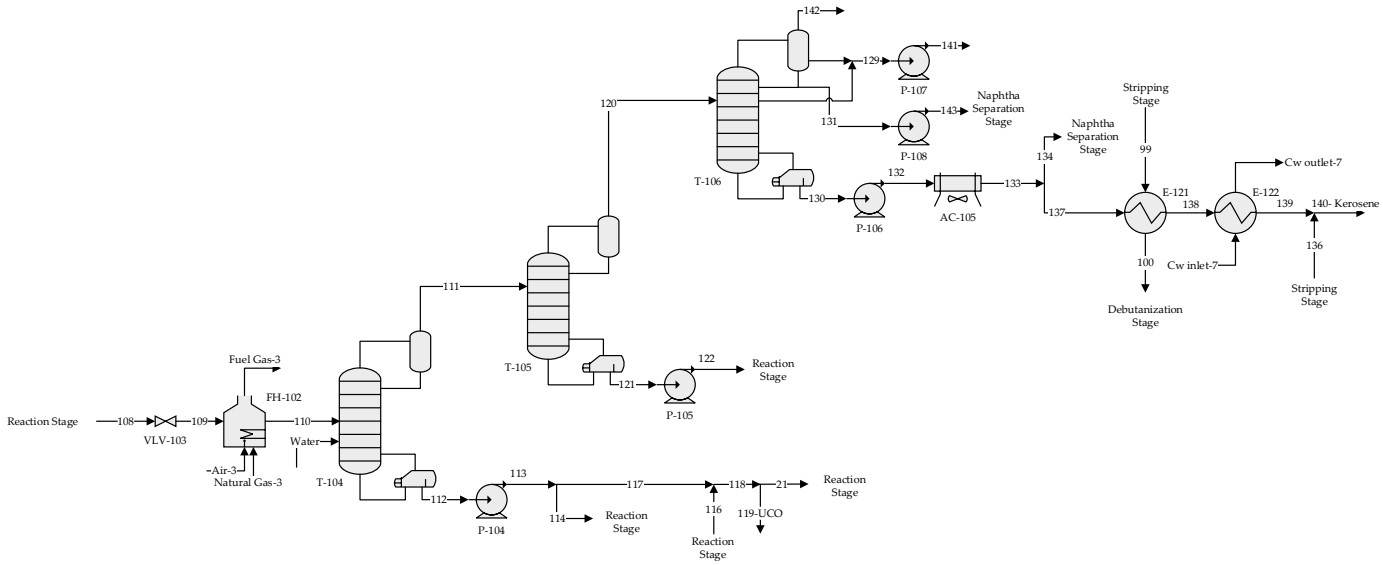

Figure 6. Fractionation stage of the energy-integrated gas oil hydrocracking process.

2.1.6. Naphtha Separation Stage

In the naphtha separation stage, 40,931 kg/h of naphtha is fed into the distillation column T-107 at a temperature of 97.6 °C and a pressure of 2.53 bar, where 9806 kg/h of light naphtha is obtained as the distillate and 31,093 kg/h of heavy naphtha as the bottom product; for the separation, the reboiler uses steam as the heating medium with a heat duty of 25,094 MJ/h, while the condenser operates with cooling water and a heat duty of 22,531 kcal/h, as illustrated in Figure 7.

From an inventory perspective, the simulated facility contains an Inside Battery Limit (ISBL) inventory of 2838.3 t and an Outside Battery Limit (OSBL) inventory of 488.4 t. These large material inventories, combined with the severe operating conditions and structural complexity of the unit, form the basis for the subsequent evaluation of the Inherent Safety Index (ISI).

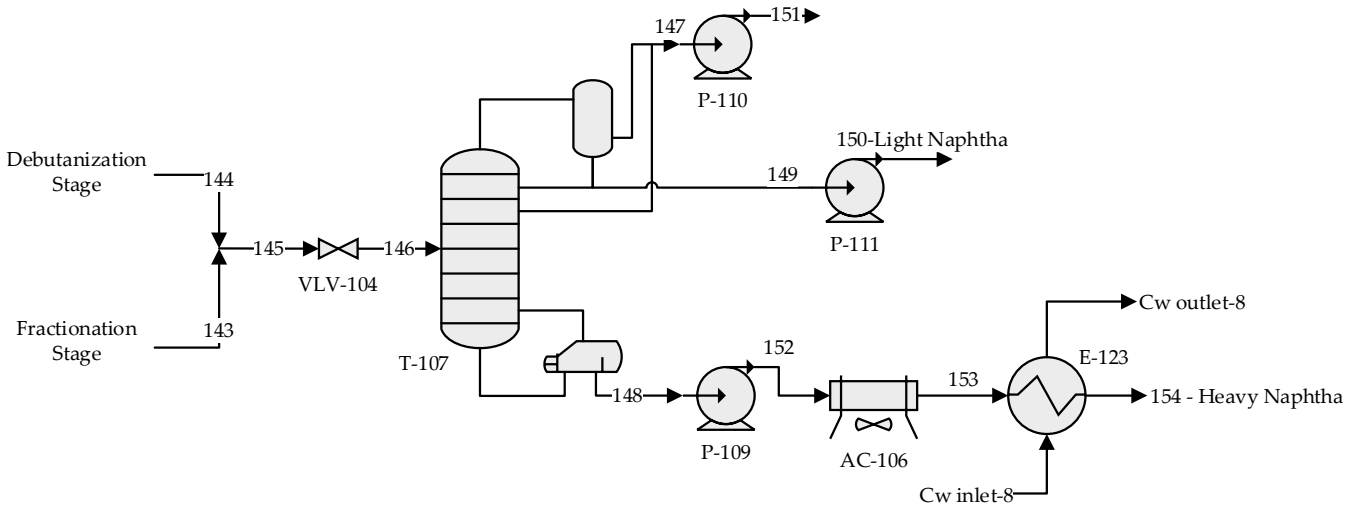

Figure 7. Naphtha separation stage of the energy-integrated gas oil hydrocracking process.

2.2. Inherent Safety Index Evaluation

The Inherent Safety Index (ISI), proposed by Heikkilä [11], constitutes a tool for evaluating the safety level of a chemical process based on its intrinsic characteristics, without relying on additional control or protection measures. The methodology integrates factors related to the properties of the substances involved, the reactive phenomena inherent to the process, and the operating conditions established at each stage. The Total Inherent Safety Index (I_{TI}) is determined as the sum of the index associated with chemical substances (I_{ch}) and the index related to the process (I_{ps}), as expressed in Equation (1). It is important to emphasize that, for the determination of the subindices, the chemical substance or process condition that results in the highest subindex is taken into consideration [15]. This conservative criterion ensures that the most critical hazard is adequately represented and that the inherent risk of the process is not underestimated.

$$I_{TI} = I_{ch} + I_{ps} \quad (1)$$

The subindex associated with chemical substances is calculated by considering several parameters inherent to the behavior of the compounds involved. These include the characteristics of the main reaction, the heat released by secondary reactions, potential chemical interactions, as well as flammability, explosiveness, toxic exposure, and corrosivity criteria. Together, these factors allow for a comprehensive assessment of the intrinsic hazardousness of the substances. Equation (2) presents the mathematical expression used to determine this index.

$$I_{ch} = I_{RM} + I_{RS,MAX} + I_{INT} + I_{FL} + I_{EX} + I_{TOX} + I_{COR} \quad (2)$$

where I_{RM} represents the subindex of the heat of the main reaction, $I_{RS,max}$ corresponds to the subindex associated with the maximum heat released by secondary reactions, I_{INT} denotes the chemical interaction subindex, I_{FL} is the flammability subindex, I_{EX} is the explosiveness subindex, I_{TOX} is the toxic exposure subindex, and I_{COR} is the corrosivity subindex. Subsequently, Table 3 presents the classification of the subindices that constitute this indicator, together with the score ranges assigned to each of them [11].

In its first part, the method focuses on hazards arising from the chemical nature of the system, which are expressed through subindices related to reaction heat, the presence of hazardous substances, and potential undesirable interactions between chemicals [16]. The thermal behavior of reactions is a fundamental element within the ISI framework, since the severity of an accidental event is often directly linked to the amount of energy

released. To assess this aspect, the heat of reaction is determined using Hess's Law. The same rationale is applied to secondary reactions that may occur within the process, using the side reaction with the highest energy release as the representative case [17]. Figure 8 presents the subindices as a function of the reaction heat [11].

Table 3. Score ranges for the inherent chemical safety subindex.

Chemical Inherent Safety Index (Ich)	Score Range
Heat of main reaction (I_{RM})	0–4
Heat of side reaction, max ($I_{RS,MAX}$)	0–4
Chemical interaction (I_{INT})	0–4
Flammability (I_{FL})	0–4
Explosiveness (I_{EX})	0–4
Toxic exposure (I_{TOX})	0–6
Corrosiveness (I_{COR})	0–2

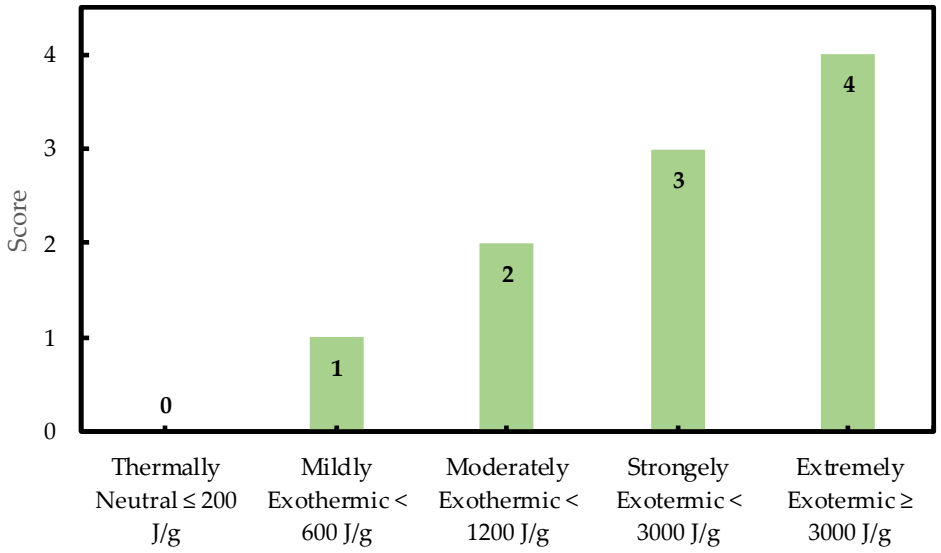

Figure 8. Determination of reaction heat for the I_{RM} and I_{RS} subindices.

In addition to reactive behavior, the ISI incorporates a specific subindex to evaluate undesirable chemical interactions between process substances. For its determination, a systematic review of the safety data sheets (SDSs) of each substance involved is carried out, and, complementarily, a chemical compatibility chart is developed to identify potentially hazardous combinations [18]. This methodology makes it possible to anticipate phenomena such as incompatibilities, catalyzed decompositions, unintended reactions, or material degradation, which can significantly increase the inherent risk of the process if not adequately considered during the design stage. Table 4 presents the score ranges as a function of chemical interaction severity [11].

Table 4. Determination of the chemical interaction subindex.

Chemical Interaction	Score Range
Heat formation	1–3
Fire	4
Formation of harmless, non-flammable gas	1
Formation of toxic gas	2–3
Explosion	4
Rapid polymerization	2–3
Soluble toxic chemicals	1

The method also considers the hazard associated with the individual properties of the substances used in the process. In particular, the flammability subindex is determined based on the flash point and the boiling point of each compound. This classification makes it possible to assign the inherent risk level associated with each substance according to its ability to initiate and sustain combustion [19]. Figure 9 presents the corresponding scores as a function of the flammability degree of the substances evaluated [11].

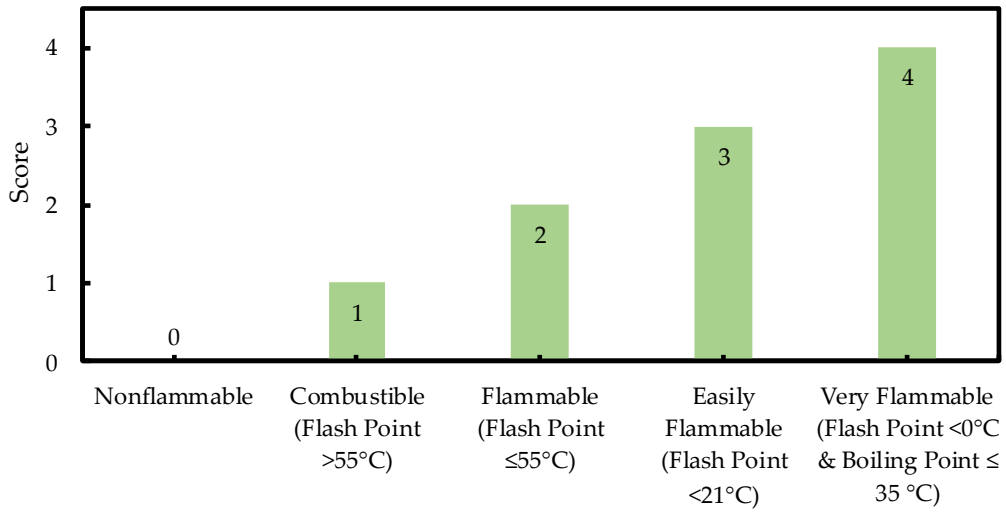

Figure 9. Determination of the flammability subindex.

With regard to explosiveness, the ISI adopts as its primary criterion the range between the lower explosive limit (LEL) and the upper explosive limit (UEL). A wider interval indicates that the substance is capable of forming flammable mixtures over a broader concentration range [20], which results in a higher score within the index, as it increases the likelihood of encountering hazardous conditions during operation. Figure 10 presents the scores assigned as a function of the explosive limits of the substances evaluated [11].

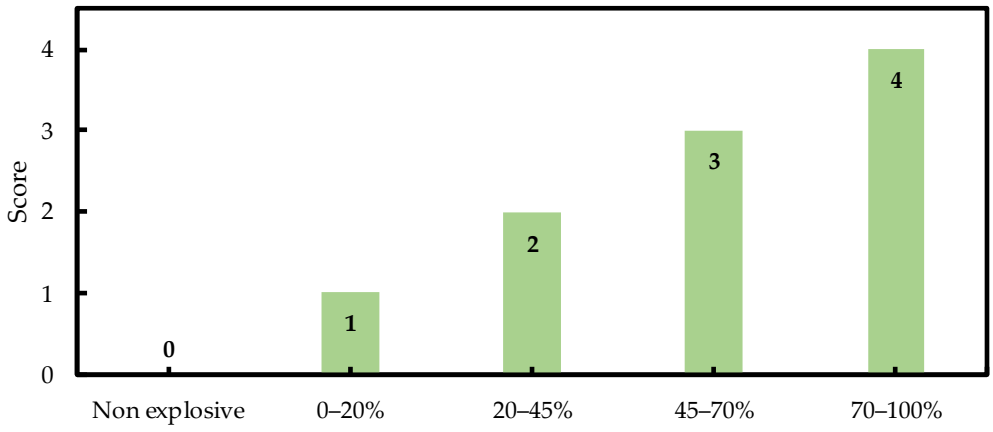

Figure 10. Determination of the explosiveness subindex.

Toxicity is evaluated using occupational exposure limit values (TLVs), which are available for most substances used in industry. Within this subindex, compounds with lower TLV values, and, therefore, greater potential harm to human health, are assigned higher scores. For this purpose, the Threshold Limit Value–Time-Weighted Average (TLV-TWA) is used, which corresponds to the time-weighted average concentration over an 8 h workday and a 40 h workweek [21], below which adverse health effects are not expected to occur, even after repeated exposures throughout a working lifetime. In accordance with the ISI approach, the classification is performed by considering the most unfavorable TLV

value among the substances analyzed. Figure 11 presents the scores assigned for toxic exposure as a function of the toxicity level derived from the TLV-TWA [11].

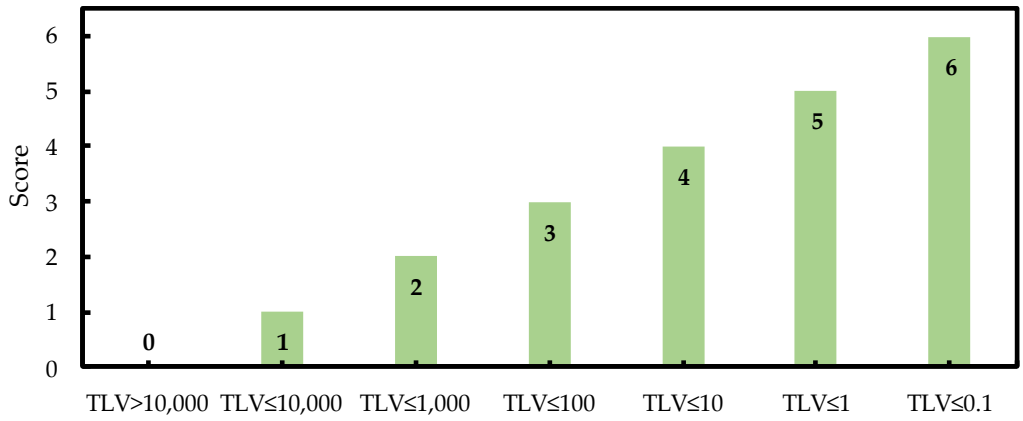

Figure 11. Determination of the toxic exposure subindex.

The corrosive potential is estimated based on the type of construction material required for the safe operation of the process. In general, a system that can operate using carbon steel is considered less severe than one that requires stainless steels or special materials resistant to highly aggressive environments. This classification reflects the intensity of chemical attack that process substances may exert on exposed materials [22]. Figure 12 presents the scores assigned for corrosivity, differentiated according to the level of resistance required from the construction materials [11].

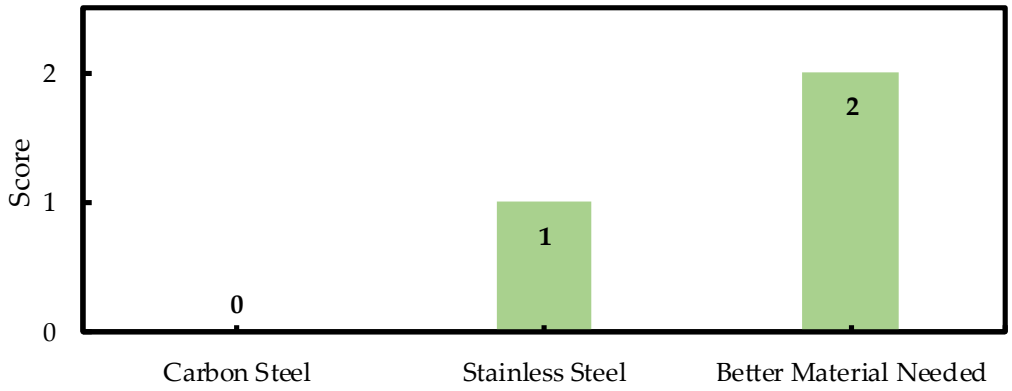

Figure 12. Determination of the corrosivity subindex.

The second part of the Inherent Safety Index (ISI) focuses on the identification and evaluation of hazards associated with the process configuration and its fundamental operating parameters. Unlike the first section, which is primarily oriented toward the intrinsic properties of the substances involved, this stage of the analysis examines how design and operational decisions directly influence the inherent risk level of the system. Factors such as operating temperature and pressure conditions, the type of equipment employed, and the overall process structure determine the magnitude of stored energy, operational complexity, and the probability of failures, thereby constituting critical elements for process safety. In this context, the evaluation not only allows the inherent hazardousness of the process to be assessed but also enables the identification of opportunities to reduce risk from the design stage, in accordance with the principles of inherent safety. Based on the above, the process Inherent Safety Index is calculated as the sum of the subindices associated with

the system configuration and operation, as expressed in Equation (3), the ion of the toxic exposure subindex.

$$I_{ps} = I_I + I_T + I_P + I_{EQ} + I_{ST} \quad (3)$$

where I_I represents the inventory subindex, I_T corresponds to the temperature subindex, I_P to the pressure subindex, I_{EQ} to the equipment safety subindex, and I_{ST} to the safe process structure subindex.

Table 5 summarizes the scoring ranges assigned to each subindex composing the inherent process safety index, which are used to quantify the contribution of inventory, operating conditions, equipment characteristics, and process structure to the overall inherent risk of the system. These ranges provide a consistent basis for evaluating and comparing alternative process configurations according to the ISI methodology [11].

Table 5. Score ranges for the process inherent safety subindices.

Process Inherent Safety Subindices	Score Range
Inventory (I_I)	0–5
Process Temperature (I_T)	0–4
Process Pressure (I_P)	0–4
Equipment Safety (I_{EQ})	
ISBL	0–4
OSBL	0–3
Safe Process Structure (I_{ST})	0–5

The inventory of ISBL and OSBL equipment is determined based on the mass flow rate of the inlet streams to each unit, considering a residence time of one hour; for this calculation, equipment with low residence times, such as pumps, compressors, and air coolers, is excluded. The classification between ISBL and OSBL equipment is established using a representative process scheme, in which units directly involved in the process are defined as ISBL, while those intended for the storage of raw materials or products are classified as OSBL [23]. This approach enables the quantification of the risk associated with the amount of material available at each stage of the process. Table 6 presents the classification used for the determination of the inventory subindex [11].

Table 6. Determination of the inventory subindex.

Inventory ISBL	Inventory OSBL	Score Range
0–1 t	0–10 t	0
1–10 t	10–100 t	1
10–50 t	100–500 t	2
50–200 t	500–2000 t	3
200–500 t	2000–5000 t	4
500–1000 t	5000–10,000 t	5

Process temperature constitutes a key indicator of the level of internal energy stored within the system. Elevated temperatures may promote undesired reactions, accelerate material degradation, and compromise thermal stability, whereas cryogenic conditions introduce risks associated with material embrittlement and thermal shock failures [24]. In both cases, significant deviations from ambient conditions increase the inherent risk score of the process due to the higher likelihood of mechanical failures or hazardous phenomena. Figure 13 presents the classification used to determine the process temperature subindex [11].

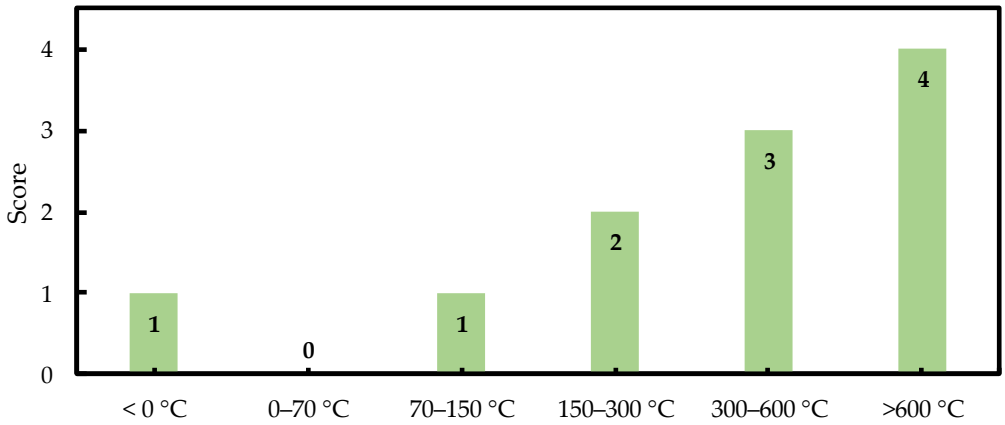

Figure 13. Determination of the process temperature subindex.

Operating pressure constitutes a direct indicator of the mechanical demands imposed on process equipment. Elevated pressure levels increase both the likelihood and severity of structural failures, catastrophic leaks, and sudden releases of stored energy [25]. Consequently, processes operating at high pressures are assigned a higher risk weighting, particularly when such conditions are combined with hazardous fluids or extreme temperatures that may compromise system integrity. Figure 14 presents the classification used to assign the pressure subindex score based on characteristic process pressure values [11].

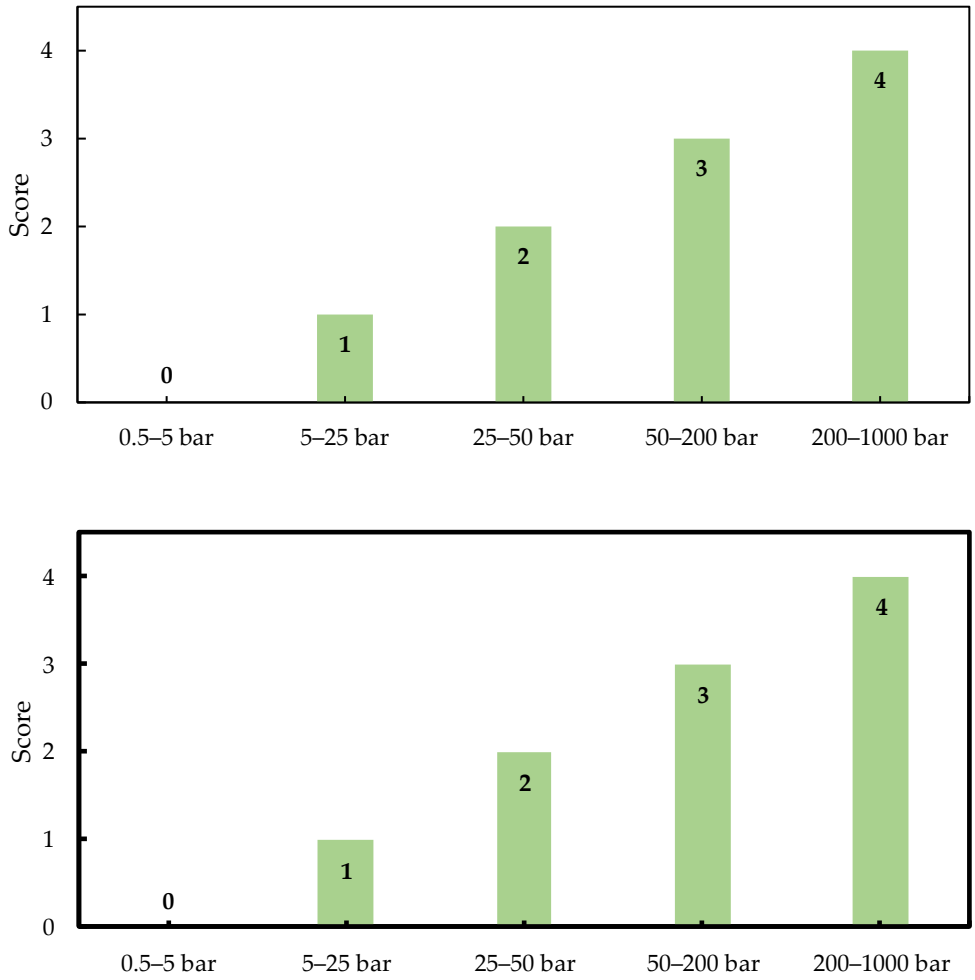

Figure 14. Determination of the process pressure subindex.

To reflect the contribution of equipment design to the inherent risk of the process, the method incorporates a subindex that evaluates the intrinsic safety of the main equipment, distinguishing between units that are more susceptible to mechanical or dynamic failures, such as pumps and compressors, and structurally more stable equipment, such as static vessels, since not all units contribute equally to the overall system risk [26]. In particular, equipment located within the battery limits (ISBLs, Inside Battery Limits) constitutes the operational core of the process, as it concentrates essential unit operations and operates under demanding pressure, temperature, or dynamic conditions that may amplify risk if the design, selection, or configuration is inadequate. Therefore, the specific evaluation of equipment safety is fundamental for identifying vulnerabilities associated both with the properties of the substances handled and with the engineering decisions adopted during the design stage. Table 7 presents the score assigned to the equipment safety subindex according to the type of ISBL equipment present in the process [11]; additionally, the method establishes that the final equipment score corresponds to the maximum value obtained between the ISBL and OSBL subindices, in order to represent the intrinsically most unfavorable scenario.

Table 7. Determination of the ISBL equipment safety subindex.

Equipment	Score
Equipment that handles non-flammable and non-toxic materials.	0
Heat exchangers, pumps, towers, and drums	1
Air coolers, reactors, and high-risk pumps	2
Compressors and high-risk reactors	3
Furnace and fire heaters	4

Equipment located outside the battery limits (OSBLs, Outside Battery Limits) performs essential support functions for plant operation, although it does not participate directly in the main process train. This equipment includes storage systems, industrial service supply, utilities, and effluent handling facilities. Although their interaction with the process operating conditions is less immediate than that of ISBL equipment, their performance has a decisive influence on the overall system reliability and on the plant's ability to respond to operational deviations. Therefore, their evaluation within the index must consider the robustness of utility systems, the stability of supply conditions, and the effectiveness with which these auxiliary units can prevent the propagation of failures toward the ISBL area. Consequently, the assessment of OSBL equipment does not represent a secondary aspect but rather a key component in ensuring an integrated and consistently safer process design. Table 8 presents the score assigned to the subindex according to the type of equipment located outside the battery limits [11].

Table 8. Determination of the inventory subindex for OSBL equipment.

Equipment	Score
Equipment that handles non-flammable and non-toxic materials	0
Atmospheric storage tanks and pumps	1
Cooling towers, compressors, purge systems, pressurized or refrigerated storage tanks	2
Boilers and furnaces	3

The safe process structure subindex is used to evaluate the inherent safety of a process configuration based on the available knowledge of its operational performance. Within this methodology, process structures are classified into six discrete levels, with scores

ranging from 0 to 5, where lower values represent recommended or standardized configurations with a favorable safety record, while higher values correspond to structures associated with documented accident histories. The assignment of the subindex value is based on information derived from good engineering practices, operational experience, design recommendations, and historical accident analyses. The resulting value is subsequently integrated with the other subindices of the Inherent Safety Index, enabling the comparison of process alternatives and supporting the selection of safer design concepts during the early stages of process development, in accordance with the approach proposed by Heikkilä et al. [11]. The procedure for determining the process structure subindex is illustrated in Figure 15.

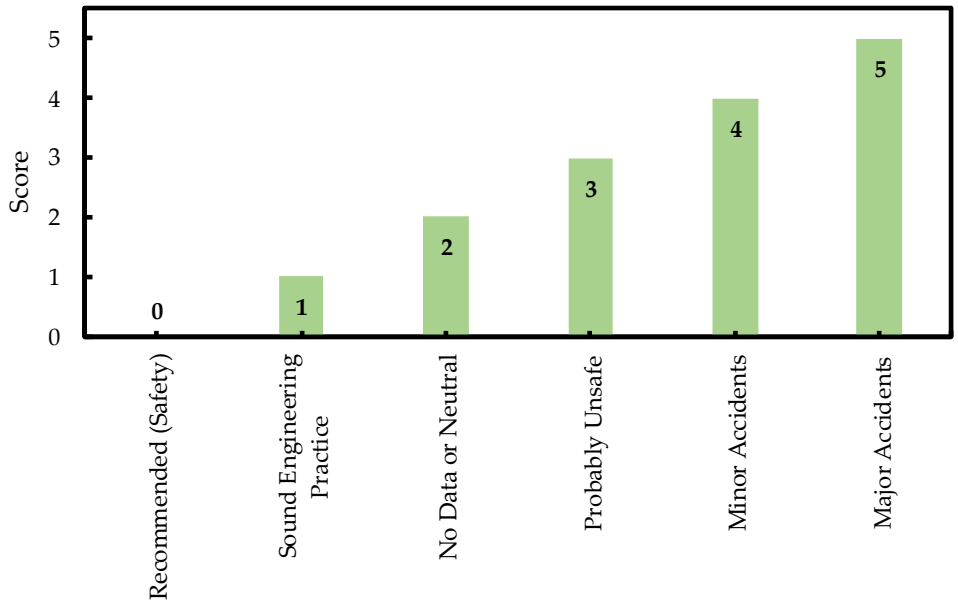

Figure 15. Determination of the process structure subindex.

3. Results and Discussion

3.1. Chemical Process Subindices

The subindices related to the chemical substances involved in the energy-integrated hydrocracking process are presented in Figure 16. The first evaluated subindex corresponds to I_{RM}, for which the main reaction considered is the hydrocracking of heneicosane to produce heptadecane and ethane. This reaction takes place in reactors HCR-100 and HCR-101 and presents a heat of reaction of −2218.5 J/g. Due to the value of the heat of reaction associated with this process, a score of 2 is assigned to this subindex, indicating the need to implement appropriate thermal control and operational safety measures in the involved equipment.

The $I_{RS,MAX}$ subindex is determined based on the hydrotreating reaction of cyclohexanecarboxylic acid, which presents a heat of reaction of −11,892.6 J/g. This value indicates a high potential for thermal risk under abnormal operating conditions; therefore, in this case, a score of 4 is assigned to the subindex, corresponding to the maximum level of the indicator.

The chemical interaction is a key parameter in the evaluation of inherent process safety, as it reflects the potential risks associated with hazardous interactions between substances. In this study, the I_{INT} subindex received the maximum score of 4, indicating a significant potential for fires or explosions under extreme conditions where fuels, oxidizing agents, and ignition sources may coexist. This evaluation is supported by the chemical compatibility chart presented in Figure 17, which reveals critical interactions among the substances

involved in the process. In particular, the chart shows that methyldiethanolamine exhibits an incompatible interaction with hydrogen sulfide, characterized by heat and gas generation, potentially intense or explosive reactions, and toxic effects, while its interaction with hydrogen requires caution due to flammability and associated hazards. These findings, obtained from the CAMEO Chemicals database, justify the assignment of the maximum value to the I_{INT} subindex and confirm the presence of relevant chemical interaction risks within the system.

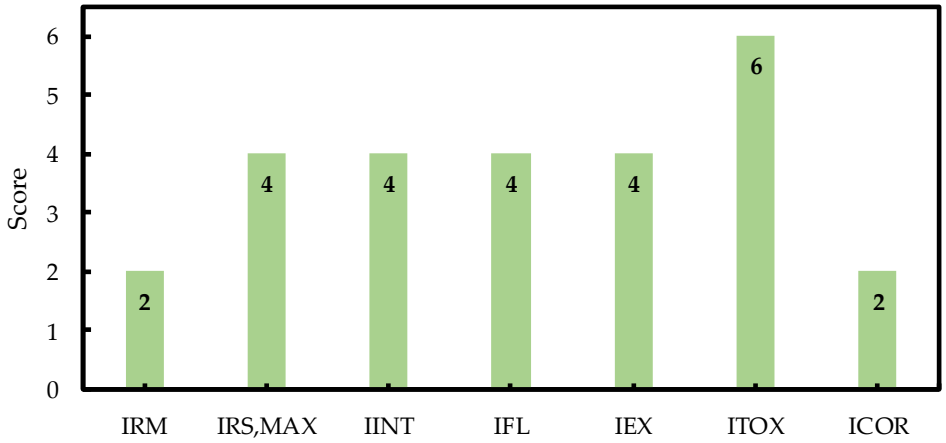

Figure 16. Distribution of inherent chemical safety subindex scores.

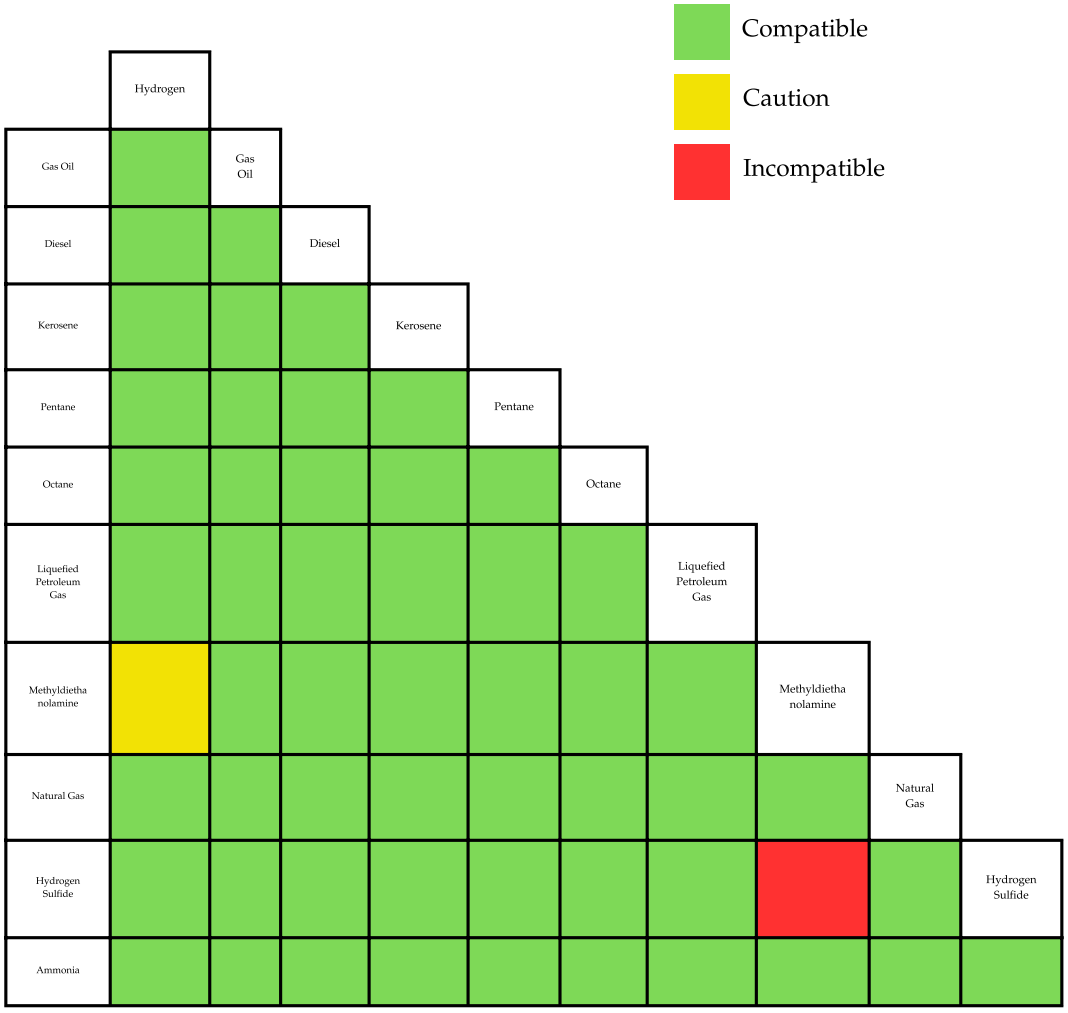

Figure 17. Chemical compatibility chart for the energy-integrated gas oil hydrocracking process.

The flammability subindex (I_{FL}) was assigned a value of 4, mainly due to the presence of highly flammable hydrocarbons such as methane, butane, and i-pentane. Among these substances, methane represents the most critical compound under the flammability criterion, as it exhibits a flash point of −188 °C and a boiling point of −161.5 °C, characteristics that favor rapid vaporization and significantly increase the probability of ignition under leak or accidental release scenarios. The results of this analysis for the key substances are presented in Table 9, based on physicochemical data obtained from Safety Data Sheets (SDSs). From a sustainability perspective, high flammability increases the likelihood and potential severity of fire-related incidents, which may lead to environmental damage, infrastructure loss, and risks to workers and nearby communities. Large-scale fire events can generate secondary emissions, including greenhouse gases and particulate matter, thereby amplifying environmental externalities.

Table 9. Determination of the flammability subindex.

Chemical Substance	Flash Point, °C	Boiling Point, °C	Flammability Type	Score I_{FL}
Butane	−60	−0.5	Very flammable	4
i-pentane	−40	35	Very flammable	4
Methane	−188	−161.5	Very flammable	4
Octane	13	126	Easily flammable	3

Regarding explosivity, hydrogen represents the most critical substance in the system due to its wide explosive limits in air, with a lower explosive limit (LEL) of 4% and an upper explosive limit (UEL) of 75%, corresponding to an explosive range of 71%. This extensive flammability range significantly increases the likelihood of forming explosive atmospheres, particularly in confined spaces or areas with limited ventilation, thereby emphasizing the need for appropriate detection, ventilation, and control systems. Consequently, these characteristics justify the assignment of the maximum value of 4 to the explosivity subindex (I_{EX}). Beyond process safety considerations, hydrogen explosivity also has important sustainability implications. Although hydrogen is not toxic, accidental releases under high-pressure conditions can lead to severe fires or explosions, generating overpressure waves, structural damage, and potential secondary releases of hazardous substances. Such events may extend beyond plant boundaries, posing risks to workers, nearby communities, and surrounding infrastructure.

Furthermore, the toxic exposure subindex (I_{TOX}) reached the maximum score of 6, mainly due to the presence of arsenic retained in the catalysts from the gas oil charge, which represents a problem because it poisons the catalysts and is a toxic substance [27], characterized by a very low TLV-TWA value reported by the Occupational Safety and Health Administration (OSHA). This result highlights the potential severity of both acute and chronic health effects associated with catalyst handling, disposal, and accidental exposure. From an inherent safety perspective, reducing arsenic content in the feedstock prior to entering the process unit would lower the toxicological hazard at its source, thereby improving the intrinsic safety index and simultaneously reducing occupational risk.

The corrosivity subindex (I_{COR}) was assigned the maximum value of 2 due to the presence of corrosive species, such as hydrochloric acid, naphthenic acids, and sulfur compounds, which may accelerate equipment degradation and increase the likelihood of loss of containment. In particular, carbon steel is highly susceptible to hydrogen attack when exposed to temperatures above 205 °C [28]. Additionally, the presence of hydrogen sulfide promotes sour corrosion, a critical degradation mechanism in petroleum processing environments, characterized by severe damage such as pitting, cracking, wall thinning, and structural failure in pipelines, vessels, and metallic components [29]. According to in-

dustry studies, hydrogen sulfide is responsible for approximately 40% of corrosion-related failures in the oil and gas sector [30], highlighting its dominant role in equipment degradation. These combined degradation mechanisms significantly increase the probability of mechanical failure and loss of containment, emphasizing the necessity of employing corrosion-resistant materials and appropriate metallurgical selection.

The main physicochemical and hazard-related properties of the chemical substances considered in this subindex and used for the determination of the explosivity and corrosion-related subindices are summarized in Table 10 based on information obtained from scientific articles and the ChemPub database.

Table 10. Determination of explosivity subindex.

Chemical Substance	LEL	UEL	UEL-LEL	TLV, ppm	Material Construction Required	Reference
Hydrogen	4%	75%	71%	Non-Toxic	Stainless Steel	[31–33]
Arsenic	There is no information	There is no information		0.01	Better Material Needed	[34]
Hydrogen Sulfide	4%	44%	40%	1	Better Material Needed	[31,35,36]

3.2. Process Safety Subindices

Figure 18 presents a schematic layout of the most representative equipment in the energy-integrated hydrocracking process, taking into account the compatibility chart shown in Figure 17 as the technical criterion for the placement of storage units.

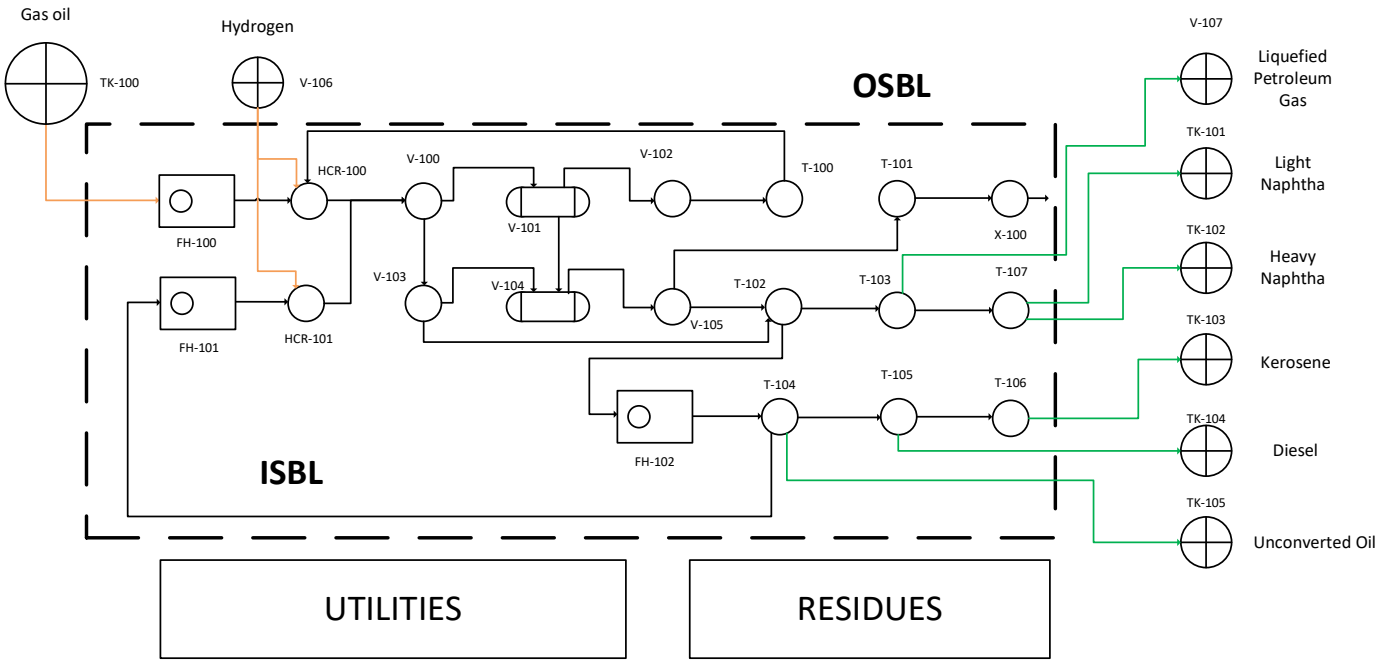

Figure 18. Process equipment schematic for ISBL and OSBL areas.

For the calculation of the ISBL equipment inventory, only process units characterized by a significant material hold-up were considered. These units comprised reactors, pressure vessels, absorption columns, the fractional distillation column, component splitters, and the combustion furnace. The inventory associated with each unit was estimated based on its operating conditions and an assumed residence time of one hour to simplify the calculation at this conceptual stage, after which the individual contributions were aggregated to

determine the total ISBL inventory. The results of this assessment indicate a total ISBL inventory of 2838.3 tons, as detailed in Table 11, which corresponds to an ISBL inventory subindex value of 5, representing the highest classification within the adopted inherent safety methodology.

Table 11. ISBL equipment inventory results.

Equipment ISBL	Inventory, t
Hydrocracking Reactor (HCR-100)	110.6
Hydrocracking Reactor (HCR-101)	185.4
Absorption Column (T-100)	141.1
Absorption Column (T-101)	6.1
Distillation Column (T-102)	412.9
Distillation Column (T-103)	16.7
Distillation Column (T-104)	393.7
Distillation Column (T-105)	199.2
Distillation Column (T-106)	92.6
Distillation Column (T-107)	40.9
Separator (V-100)	495.1
3 Phase Separator (V-101)	204.1
Separator (V-102)	83.7
Separator (V-103)	316.5
3 Phase Separator (V-104)	132.8
Separator (V-105)	3.6
PSA Splitter Component (X-100)	
Total	2838.3

In contrast, the OSBL inventory calculation was restricted exclusively to raw material and product storage equipment, including fuel oil, hydrogen, LPG, light naphtha, heavy naphtha, kerosene, diesel, and unconverted petroleum oil (UCO), as these units represent the main accumulation of material Outside Battery Limits. A uniform residence time of one hour was assumed as a methodological criterion to ensure consistency in the inventory estimate. The results obtained indicate a total stored mass of 488.4 tons, as summarized in Table 12, corresponding to an OSBL inventory subindex of 2. However, because the ISBL inventory subindex was higher, the maximum subindex of 5 was ultimately adopted for the overall inherent safety assessment, in accordance with the conservative criteria established by the methodology. It is important to emphasize that the evaluation of this subindex is fundamental, as a reduction in process inventory directly contributes to a lower ISI value. Decreasing the quantity of hazardous substances, particularly flammable, explosive, toxic, and corrosive materials, not only reduces the overall hazard intensity within the system but also minimizes the potential environmental and social impact in the event of accidental releases [37]. From a sustainability perspective, limiting hazardous inventories decreases the magnitude of possible externalities, enhances community safety, and strengthens the resilience of industrial operations by reducing the consequences associated with major incidents.

The pressure subindex (I_P) was assessed at 3, associated with a maximum operating pressure of 166.8 bar recorded in the hydrogen outlet stream of compressor K-103. This equipment is part of the hydrogen recovery and replenishment stage, in which the gas is compressed before being redistributed to the process units, thus constituting the most severe pressure condition within the overall system. Because this section concentrates the highest level of stored energy and, therefore, the greatest mechanical stress on the equipment, the assigned subindex value is justified. According to the applied methodology, a decrease in the hydrogen operating pressure would imply a reduction in ISI [38], since

the equipment would operate under lower mechanical demands and, consequently, with a lower risk of overpressure failures, extending the vessel's service life [39].

Table 12. OSBL equipment inventory results.

Equipment OSBL	Inventory, t
Gas Oil Storage Tank	243.6
Light Naphtha Storage Tank	9.8
Heavy Naphtha Storage Tank	31.1
Kerosene Storage Tank	60.5
Diesel Storage Tank	106.6
Hydrogen Storage Vessel	32.9
LPG Storage Vessel	3.7
Total	488.4

Similarly, the temperature subindex (I_T) was classified within the upper range due to a maximum operating temperature of 456.1 °C in the fractionation section, specifically in the distillation column T-104, where high temperatures are required to ensure effective hydrocarbon separation; this justifies the assigned value of 3, as it represents the most thermally severe condition in the process. Such elevated temperatures intensify mechanical and metallurgical stresses, accelerating degradation mechanisms, such as thermal fatigue, oxidation, and strength reduction [28,40], while also increasing occupational risks, particularly burn hazards associated with hot surfaces and insufficient insulation. Consequently, a reduction in this temperature subindex would not only decrease mechanical stress on the equipment but also generate social benefits by lowering workers' exposure to extreme temperatures and improving operational safety conditions.

In this case, an equipment safety subindex value of 4 was assigned based on the high probability of failure associated with critical equipment and the potential consequences arising from loss of containment or operational malfunction under severe operating conditions. This assessment is justified by the presence, within the ISBL, of equipment whose operation requires strict and continuous control due to the high pressures and temperatures involved in the process. In particular, the combustion furnaces responsible for the preheating of gas oil feed streams to the hydrocracking reactors were identified as critical units. These furnaces act as potential ignition sources and are exposed to extreme thermal conditions, which may accelerate degradation mechanisms such as thermal fatigue, hot spot formation, and overheating failures [41]. Additionally, the reactors and associated pressurized vessels represent sensitive points in the process, where a mechanical failure could result in rapid energy releases, leading to severe consequences for overall system integrity. Consequently, the operation of the combustion furnaces within the ISBL constitutes the primary factor supporting the assignment of an equipment safety subindex of 4, reflecting the elevated level of inherent risk associated with these units.

The safe process structure was assigned the maximum score of 5 based on the severity and likelihood of structural failures observed in similar industrial units. This decision is supported by technical evidence derived from real industrial accidents, such as the incident that occurred at the BP Grangemouth refinery hydrocracking unit (Scotland) in 1987 [42]. In that event, a loss of liquid level in a high-pressure separator allowed gas carryover into a lower-pressure system, triggering an explosion that destroyed equipment and resulted in fatalities. This accident demonstrated that, even in facilities with advanced designs, operational transitions and poorly controlled separation systems can compromise structural integrity and lead to catastrophic failures. In this context, the assignment of the maximum score is not arbitrary; rather, it reflects the fact that the analyzed process structure exhibits similar vulnerability conditions, including the handling of high pressures,

the presence of critical equipment whose failure may trigger rapid energy releases, and operational dependencies among reactors, separators, and piping systems. Historical evidence confirms that these elements make mechanical integrity and structural design decisive factors in the overall process risk, thereby justifying the assigned value. Figure 19 presents the distribution of the process inherent safety subindex for the energy-integrated hydrocracking process.

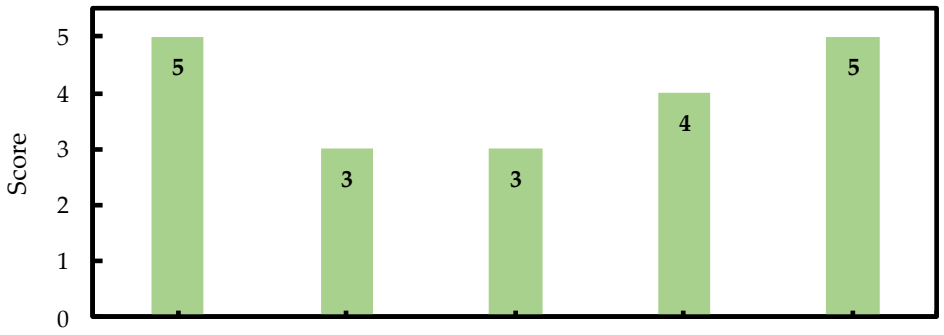

Figure 19. Distribution of process inherent safety subindex scores.

The application of the Inherent Safety Index (ISI) to the analyzed hydrocracking process resulted in a total value of 46, indicating a high level of inherent risk according to the criteria established by the methodology. This value reflects the combined contribution of the chemical substances subindex, which accounted for 26 points, and the process-related safety subindex, with a value of 20 points. The overall ISI results are presented in Figure 20. These findings demonstrate that, even in mature industrial processes that are extensively optimized from an operational perspective, the simultaneous presence of hazardous substances, large inventories, severe pressure and temperature conditions, and a complex process structure generates a substantial intrinsic risk that cannot be effectively mitigated solely through active safety systems or administrative measures.

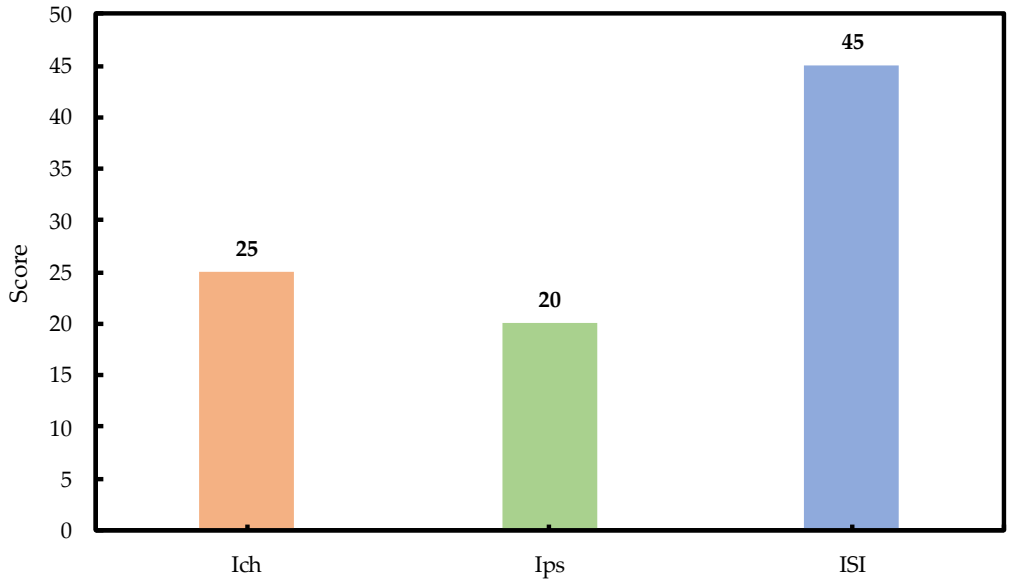

Figure 20. Inherent Safety Index (ISI) results.

Subsequently, a sensitivity assessment was performed to quantify the extent to which operating temperature and pressure conditions impact the intrinsic safety performance of the process. As shown in Figure 21, the maximum temperature and pressure were varied independently to assess their direct contribution to ISI. This approach isolates the individual

effect of each parameter, without considering process interactions or performance-related constraints such as conversion, selectivity, or thermal efficiency. The analysis indicates that, under purely theoretical conditions, both parameters could reduce the ISI by up to three points. However, such a reduction would require decreasing the maximum operating temperature from 456.4 °C to 70 °C, or the maximum pressure from 166.8 bar to 5 bar. These conditions are not physically feasible for industrial hydrocracking operation and should, therefore, be interpreted only as theoretical lower-bound scenarios used to evaluate the sensitivity of the ISI methodology. Consequently, the results do not constitute practical operating recommendations but rather illustrate the strong influence of operating severity on the overall Inherent Safety Index. Significant improvements in intrinsic safety would require alternative design strategies and a detailed assessment of their impact on reactor performance, fractionation efficiency, and product conversion.

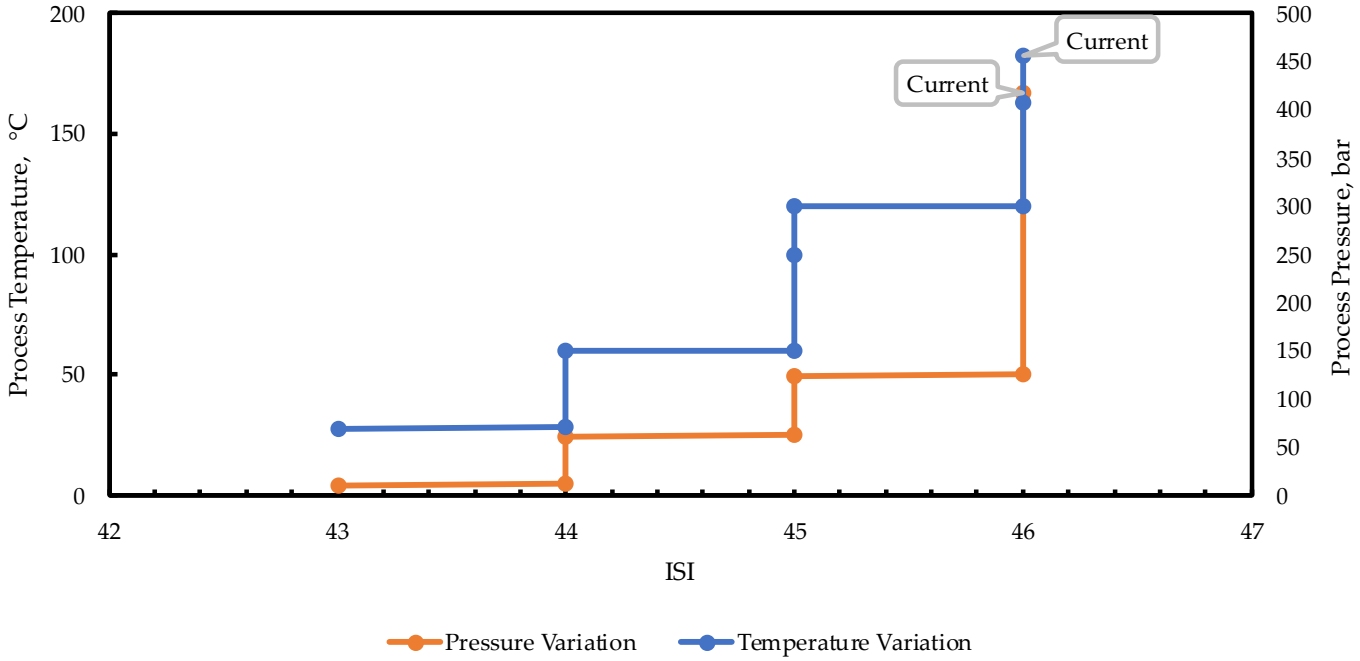

Figure 21. Sensitivity analysis.

Finally, the comparative inherent safety assessment, summarized in Table 13, shows that the energy-integrated hydrocracking process presents higher intrinsic risks than the PVC process, mainly due to its more severe operating conditions, reaction complexity, and toxicity. Hydrocracking operates at 456.4 °C and 166.8 bar (temperature and pressure subindices of 3 and 3), whereas the energy-integrated PVC process operates under safer conditions (250 °C and 13.7 bar), with subindices of 2 and 1 [43]. In addition, PVC does not involve secondary reactions ($I_{RS,MAX}$ = 0) [17], while hydrocracking includes a hydrotreating reaction that contributes a secondary reaction subindex of 4. Although both hydrocracking and mass–energy integrated PVC present similarly large inventories (I_I = 5) [44], toxicity represents a key difference: hydrocracking has a higher toxicity (I_{TOX} = 6) due to potential arsenic in catalysts (TLV–TWA = 0.01 ppm), whereas vinyl chloride is the most hazardous compound in PVC (TLV–TWA = 1 ppm), resulting in I_{TOX} of 5. Overall, the intrinsic safety differences are primarily driven by operating severity, reaction pathways, and toxicity rather than by integration strategies alone. Although hydrocracking and PVC production are fundamentally different processes, the comparison is meaningful because both systems were evaluated using the same ISI methodology. Therefore, the comparison serves as a benchmark for interpreting ISI values across different

industrial sectors and for discussing the influence of process integration strategies on inherent safety performance.

Table 13. Comparison of ISI values.

Case Study	I_{ch}	I_{ps}	ISI	Reference
Energy-Integrated Hydrocracking Process	25	20	45	This study
Case Base PVC Process	19	15	34	[17]
Energy-Integrated PVC Process	19	15	34	[43]
Mass/Energy Integrated PVC Process	19	14	33	[44]

4. Conclusions

This study demonstrates the applicability of the Inherent Safety Index (ISI) as a structured tool for evaluating, at the conceptual design stage, the intrinsic risk level of an energy-integrated hydrocracking unit based on its process flow diagram. The application of the ISI to this type of system represents a relevant contribution, as no previous studies have been reported in the literature applying this methodology specifically to energy-integrated hydrocracking processes. The obtained ISI value (46) indicates that the unit operates under high-severity conditions, driven by the combination of elevated temperatures and pressures, the presence of hydrogen and highly flammable hydrocarbons, toxic compounds associated with the catalyst, and large inventories of hazardous substances.

The analysis shows that the chemical safety subindex (26) predominates over the process safety subindex (20), indicating that the overall risk is mainly driven by the intrinsic properties of the substances involved. In particular, the most influential factors correspond to toxicity (I_{TOX} = 6), inventory magnitude (I_I = 5), and process structure (I_{ST} = 5), followed by explosivity and flammability (subindices of 4), as well as exothermicity and chemical interactions (I_{INT} = 4). Furthermore, although energy integration improves the thermal efficiency of the system, the present results indicate that toxicity, inventory magnitude, and operating severity remain the dominant contributors to the ISI. Therefore, the specific contribution of energy integration to inherent safety improvement in hydrocracking systems requires further investigation through comparison with non-integrated process configurations.

The equipment operating under high-pressure conditions in the process corresponds mainly to compressors, which are required to supply hydrogen to the hydrocracking reactors under severe operating conditions. In this context, the optimization of temperature and pressure conditions in the hydrocracking reactions is identified as a key strategy to improve the ISI value. Under optimized operating conditions, the ISI is estimated to decrease to approximately 43, representing a meaningful reduction in intrinsic risk. Accordingly, feedstock pretreatment to reduce arsenic content, minimization of hydrogen inventory in high-pressure equipment, and optimization of operating conditions in critical stages such as fractionation and hydrogen recovery constitute concrete strategies for ISI reduction. These findings highlight that effective risk mitigation must be addressed at the conceptual design stage by prioritizing structural and process configuration decisions, rather than relying exclusively on downstream protection and control systems. A limitation of this study is that the sensitivity analysis was performed exclusively from an inherent safety perspective and did not evaluate the impact of operating condition changes on conversion, product quality, or economic performance. Furthermore, future work should systematically evaluate the feasibility of reducing operating severity without compromising process performance, product conversion, or product quality.

From a sustainability perspective, reducing intrinsic risk in energy-integrated hydrocracking units has direct implications for occupational safety, protection of surrounding

communities, and mitigation of environmental impacts associated with major accidents. In particular, the reduction in inventories of flammable, explosive, and toxic substances decreases the potential magnitude of accidental releases, enhances system resilience, and limits long-term environmental and social impacts. Consequently, the integration of inherent safety principles into early design stages not only improves process safety performance but also contributes to the development of safer, more resilient, and more sustainable industrial systems throughout their life cycle.

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Data Availability Statement: Data supporting the conclusions of this study can be obtained from the corresponding author, Á.D.G.-D., upon reasonable request.

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Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

HCGO	Heavy Coker Gas Oil
I_{ch}	Index Of Chemical Substances
I_{COR}	Corrosivity Subindex
I_{EQ}	Equipment Safety Subindex
I_{EX}	Explosiveness Exposure Subindex
I_{FL}	Flammability Subindex
I_{I}	Inventory Subindex
I_{INT}	Chemical Interaction Subindex
I_{P}	Pressure Subindex
I_{PS}	Index Related to The Process
I_{RM}	Subindex of the Heat of the Main Reaction
$I_{RS,MAX}$	Subindex of Maximum Heat Released by Secondary Reactions
ISBL	Inside Battery Limit
ISI	Inherent Safety Index
I_{ST}	Process Structure Subindex
I_{T}	Temperature Subindex
I_{TI}	Total Inherent Safety Index
I_{TOX}	Toxic Exposure Subindex
LCGO	Light Cycle Gas Oil
LEL	Lower Explosive Limit
LPG	Liquefied Petroleum Gas
LPS	Low-Pressure Steam
MDEA	Methyldiethanolamine
MVGO	Medium Vacuum Gas Oil
OSBL	Outside Battery Limit
PSA	Pressure Swing Adsorption

SDS	Safety Data Sheet
TLV	Threshold Limit Value
TLV-TWA	Threshold Limit Value–Time-Weighted Average
UCO	Unconverted Oil
UEL	Upper Explosive Limit

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