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Abstract

Due to increasing environmental regulations, the chemical industry is evolving towards more efficient production, placing the petrochemical sector in a difficult situation due to its economic and environmental effects. In this regard, it is crucial to perform an environmental impact assessment of refinery processes to balance operational needs with environmental concerns. Fuels such as LPG (liquefied petroleum gas), naphtha, diesel, and kerosene, which are obtained by gas oil hydrocracking process on an industrial scale, are highly efficient, but present environmental problems due to emissions of toxic substances and greenhouse gases. The environmental assessment was carried out to address this challenge, using the Waste Reduction (WAR) algorithm methodology and the WAR GUI® computational tool. Subsequently, the environmental parameters of the chemicals involved in the process were calculated, an environmental impact assessment was performed, and the potential global and category impacts were evaluated, including Ozone Depletion Potential (ODP), Global Warming Potential (GWP), Photochemical Oxidation Potential (PCOP), and Acidification Potential (AP) within the atmospheric impacts, and Human Toxicity Potential by Ingestion (HTPI), Human Toxicity Potential by Inhalation or Dermal Exposure (HTPE), Aquatic Toxicity Potential (ATP), and Terrestrial Toxicity Potential (TTP) within the toxicological impacts. In this way, the environmental performance was analyzed focusing on the potential environmental impact (PEI) using the generation rate and output rate of various fuels in an integrated gas oil hydrocracking process, both from the mass and energy perspectives.

The results show that the process converts low-PEI feedstocks, such as gas oils, into higher-PEI products, such as kerosene, with significant PEI generation in Cases 2, considering products and waste (516,000 PEI/h) and 4, considering products, energy, and waste (519,000 PEI/h). However, due to the mass integration of wastewater effluents, the contribution of the process stages to PEI was reduced considering waste. On the other hand, the large product flow increased PEI per unit time, but reduced PEI per kilogram of product. Now, ATP (Aquatic Toxicity Potential) had the highest toxicological PEI (500,000 PEI/h); while PCOP (Photochemical Oxidation Potential) had the highest atmospheric PEI (36,300 PEI/h). Additionally, the stage that contributes the most to the production of PEI per hour is the preliminary separation stage, reaching 82.03% considering waste and 58.72% considering energy. On the other hand, natural gas was found to have lower environmental impacts compared to liquid (oil) and solid (coal) energy sources. Additionally, toxicological and atmospheric impacts showed moderate PEI values per category (positive and negative), demonstrating that an integrated gas oil hydrocracking process in terms of mass and energy presents better results in terms of environmental impacts, compared to a conventional gas oil hydrocracking plant, contributing to the sustainability of the process. Finally, when comparing this process with others, the integrated gas oil hydrocracking process in terms of mass and energy is more environmentally acceptable than biohydrogen production (12,000,000 PEI/h).

Keywords: Environmental Assessment; Waste Reduction (War) Algorithm; Potential Environmental Impact; Atmospheric And Toxicological Categories; Computer-Aided Process Engineering; Gas Oil Hydrocracking; Mass Integration; Fuels; Toxic Substances; Greenhouse Gases.

Evaluación Ambiental Usando Algoritmo de Reducción de Residuos de un Proceso de Hidrocraqueo de Gasóleo Integrado En Masa y Energía

Resumen

Debido a las crecientes regulaciones ambientales, la industria química está evolucionando hacia una producción más eficiente, colocando al sector petroquímico en una situación difícil debido a sus efectos económicos y ambientales. En este sentido, es crucial realizar una evaluación de impacto ambiental de los procesos de refinería para equilibrar las necesidades operativas con las preocupaciones ambientales. Los combustibles como el GLP (gas licuado de petróleo), la nafta, el diésel y el queroseno, que se obtienen mediante hidrocraqueo de gasóleo a escala industrial, son altamente eficientes, pero presentan problemas ambientales debido a las emisiones de sustancias tóxicas y gases de efecto invernadero. Para afrontar este desafío se realizó la evaluación ambiental, se utilizó la metodología del algoritmo de Reducción de Residuos (WAR) y la herramienta computacional WAR GUI®. Posteriormente, se calcularon los parámetros ambientales de las sustancias químicas involucradas en el proceso, se realizó una evaluación de los impactos ambientales y se evaluaron los posibles impactos globales y por categorías, incluyendo el Potencial de Agotamiento de la Capa de Ozono (ODP), el Potencial de Calentamiento Global (GWP), el Potencial de Oxidación Fotoquímica (PCOP) y el Potencial de Acidificación (AP) dentro de los impactos atmosféricos, y el Potencial de Toxicidad Humana por Ingestión (HTPI), el Potencial de Toxicidad Humana por Inhalación o Exposición Dérmica (HTPE), el Potencial de Toxicidad Acuática (ATP) y el Potencial de Toxicidad Terrestre (TTP) dentro de los impactos toxicológicos. De esta forma, se analizó el desempeño ambiental enfocándose en el potencial impacto ambiental (PEI) utilizando la tasa de generación y tasa de salida de varios combustibles en un proceso integrado de hidrocraqueo de gasóleo, tanto desde la perspectiva másica como energética.

Los resultados muestran que el proceso convierte materias primas de bajo PEI, como los gasóleos, en productos de mayor PEI, como el queroseno, con una generación significativa de PEI en los casos 2, considerando productos y residuos (516.000 PEI/h) y 4, considerando productos, energía y residuos (519.000 PEI/h). Sin embargo, debido a la integración másica de los efluentes de aguas residuales, la contribución de las etapas del proceso al PEI se redujo considerando los residuos. Por otro lado, el gran flujo de producto aumentó el PEI por unidad de tiempo, pero redujo el PEI por libra de producto. Ahora bien, el ATP (Potencial de Toxicidad Acuática) tuvo el PEI toxicológico más alto (500.000 PEI/h); mientras que el PCOP (Potencial de Oxidación Fotoquímica) tuvo el PEI atmosférico más alto (36.300 PEI/h). Adicionalmente, la etapa que más contribuye a la producción de PEI por hora es la etapa de separación preliminar, alcanzando un 82,03 % considerando los residuos y un 58,72 %, considerando la energía. Por otro parte, se encontró que el gas natural tiene menores impactos ambientales en comparación con las fuentes de energía líquida (petróleo) y sólida (carbón). Adicionalmente, los impactos toxicológicos y atmosféricos mostraron valores moderados de PEI por categoría (positivos y negativos), lo que demuestra que un proceso de hidrocraqueo de gasóleo integrado en términos de masa y energía presenta mejores resultados en términos de impactos ambientales, en comparación con una planta de hidrocraqueo de gasóleo convencional, contribuyendo a la sostenibilidad del proceso. Finalmente, al comparar este proceso con otros, el proceso de hidrocraqueo de gasóleo integrado en masa y energía es más aceptable desde el punto de vista ambiental que la producción de biohidrógeno (12.000.000 PEI/h). Principio del formulario

Palabras clave: *Evaluación Ambiental; Algoritmo De Reducción De Desechos (War); Impacto Ambiental Potencial; Categorías Atmosféricas Y Toxicológicas; Ingeniería De Procesos Asistida Por Computadora; Hidrocraqueo De Gasóleos; Integración Másica; Combustibles; Sustancias Tóxicas; Gases De Efecto Invernadero.*

1. Introduction

The global economy relies significantly on petroleum fuels, which are finite, environmentally detrimental, and subject to potential instability (Gebreslassie et al., 2013). These petroleum fuels come from refining crude oil through an oil refinery or a unit of such a refinery (Fan et al., 2019). In general, refineries are essential in the oil industry (Al-Rubaye et al., 2023). In this sense, in an oil refinery there may be various units such as atmospheric distillation, vacuum distillation, thermal cracking, sweetening, thermal reforming, hydrogenation, coking, solvent extraction, solvent dewaxing, catalytic polymerization, catalytic cracking, visbreaking, alkylation, isomerization, fluid catalytic cracking, deasphalting, catalytic reforming, hydrodesulfurization, inhibitor sweetening, catalytic isomerization, hydrocracking, and catalytic dewaxing (Kaiser, 2017). Now, according to the hydrocracking process, for some decades now, it has gained notable attention in the petroleum refining sector (Kamiya, 1991). This increased interest is largely attributed to the growing demand for middle distillates like kerosene and diesel in rapidly developing countries, coupled with a shift towards producing cleaner transportation fuels (Hoek et al., 1991). Hydrocracking offers an efficient way to transform heavy, sulfur-rich feedstocks into high-quality middle distillates with low sulfur and aromatic levels, alongside excellent combustion properties (Sullivan, 1985). This flexible catalytic process refines petroleum by adding hydrogen, removing impurities, and breaking down feedstocks to achieve specific boiling ranges. Hydrocracking can handle a variety of inputs, such as heavy vacuum gas oil and atmospheric gas oil, yielding diverse products from diesel to LPG, while producing fuels that comply with stringent modern environmental regulations (Gruia, 2006).

Although oil processing is one of the oldest industries, it remains a vital foundation of modern society and continues to evolve with advancements in data analysis technologies (Douet, 2020). These tools, empowered by increasing computational capabilities, offer solutions to environmental challenges associated with refineries (Abban, 2023), particularly hydrocracking units. One key issue is the composition of crude oil, which contains a mix of volatile and toxic compounds that vary depending on its source (Iplik et al., 2020). Another challenge involves sour water effluents, which are highly toxic due to their organic and inorganic content (Centeno-Bordones et al., 2021). This issue can be mitigated by integrating processes, that reduce both sour water effluents and freshwater consumption, as well as, reduce the energy consumption (El-Halwagi et al., 2003). Furthermore, the industry must address concerns such as high energy demand, emissions of harmful substances that affect human health and the environment, greenhouse gas emissions, and limited waste reuse (Wu and Liu, 2016). All these problems are included in the global difficulties that the 2030 Agenda aims to address with a set of universal objectives and goals; highlighting objectives 6 (clean water and sanitation), 7 (affordable and clean energy), 9 (industry, innovation and infrastructure), 12 (responsible production and consumption), 13 (climate action), 14 (life below water), and 15 (life on land), of the 17 Sustainable Development Goals (SDG) (FAO, 2019).

The use of techniques for quantifying environmental impacts has gained prominence in both industry and academia due to their importance in promoting sustainable practices (Mahmud et al., 2021). This evaluation is enhanced by computer-aided process engineering (CAPE), a multidisciplinary approach that manages the variables, parameters, and systems inherent in chemical processes. CAPE facilitates assessments through tools like the Waste Reduction (WAR) algorithm and its user-friendly graphical interface, GUI (Young and Cabezas, 1999). Developed by the United States Environmental Protection Agency (EPA), the WAR GUI® software provides an accessible means of evaluating the environmental impacts of chemical processes, particularly during the manufacturing phase of a product's life cycle, by streamlining key information for analysis (Sammons et al., 2009).

It is worth noting that this methodology has been implemented in various processes, including petrochemical industry processes and biorefineries, which represent the basis for implementing the WAR GUI® software in the present research; highlighting environmental assessments with the Waste Reduction (WAR) algorithm in processes such as coal gasification (Petrescu & Cormos, 2015), avocado oil production (Herrera et al., 2022), biohydrogen production (Gonzalez-Delgado et al., 2017), suspended PVC production (González-Delgado et al., 2023), biodiesel production (Rincón et al., 2014), polypropylene production (Velásquez-Barrios et al., 2018), and butylacetate production (Cardona et al., 2004). In this order of ideas, the present study aims to evaluate the environmental performance of the mass and energy-integrated gas oil hydrocracking process at an industrial scale. The WAR GUI® tool was chosen for its ability to account for both the production and generation rates of potential environmental impacts (per product unit and over time) while also assessing energy usage and the contribution of product flows to these impacts.

2. Methodology

Global process description

Figure 1 illustrates the global process flow diagram of the gas oil hydrocracking process on an industrial scale that consists of a hydrotreating and hydrocracking reaction stage, a preliminary separation stage, a make-up and recycling gas stage, and a PSA stage, and some stages of the stripping, the debutanization, the fractionation, the naphtha separation, and the make-up and recycling water stage.

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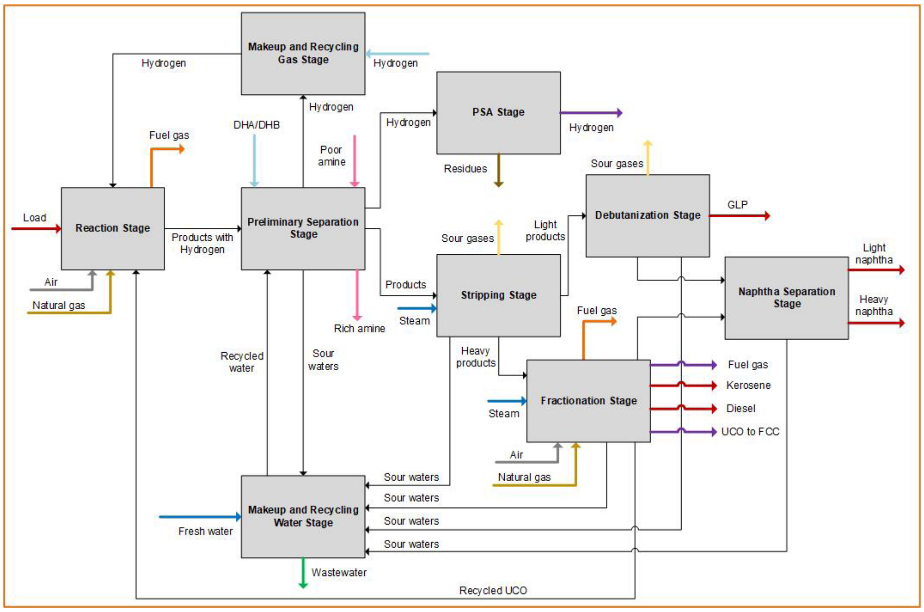
Figure 1. *Process flow diagram of mass and energy-integrated gas oil hydrocracking process.*



This topology is built from reported data from hydrocracking plants and scientific literature (García-Maza and González-Delgado, 2024). The analysis approach for the integrated gas oil hydrocracking process is through a global material balance. Therefore, in Figure 1, the global inputs and outputs of the process are illustrated. The main process feedstock (red stream) is a load of gas oil (221,147 kg/h at 112 °C and 446 kPa), other important inputs include air (grey stream), and natural gas as fuel (mustard stream) in the reaction and fractionation stage heaters, fresh water (royal blue stream) after mass integration of the process in the washing equipment in the preliminary separation stage coming from the make-up and recycling water stage, the hydrogen gas stream (light blue stream) coming from DHA/DHB in the preliminary separation stage, the poor amine streams (pink stream) in the recycle and waste gas scrubbing towers in the preliminary separation stage, the hydrogen gas stream (light blue stream) from make-up and recycling gas stage, the water vapor streams (royal blue streams) in the stripping and fractionation stages. On the other hand, the outputs focus on the flue gases (orange streams) from the heaters in the reaction and fractionation stages, the rich amine streams (pink streams) in the recycle and residual gas scrubbers in the preliminary separation stage, the residues (brown stream) and the hydrogen by-product (purple stream) from the PSA stage, the sour gas streams (yellow streams) from the stripping and debutanization stages, the LPG product (red stream) from the debutanization stage, the diesel and kerosene products (red streams) and the fuel gas and unconverted oil (UCO) to fluidized catalytic cracking by-products (purple streams) from the fractionation stage, the light and heavy naphtha products (red streams) from the naphtha separation stage, and the wastewater (green stream) in the make-up and recycling water stage. Additionally, the process goes from producing 36,568 kg/h of wastewater to 27,294 kg/h after mass integration. Finally, the process presents a product flow of 211,798 kg/h and an energy consumption of 3,129.95 GJ/h.

Environmental evaluation via WAR algorithm

The environmental assessment of the industrial-scale mass and energy-integrated gas oil hydrocracking process was performed using the WAR GUI® software, which utilizes the Waste Reduction (WAR) algorithm. This algorithm applies metrics to analyze the potential environmental impacts linked to chemical production processes. It incorporates the concept of potential environmental impact and evaluates it across eight distinct categories, grouped into two main types: toxicological impacts and atmospheric impacts (Young and Cabezas, 1999).

In this sense, the toxicological impacts are split into four categories, two human impacts and two ecological impacts. Human toxicity potential by ingestion (HTPI), Eq. (1), measures the lethal dose 50 (LD_{50}). Human toxicity potential by inhalation or dermal exposure (HTPE), Eq. (2), measures the Threshold Limit Values (TLV). Aquatic toxicity potential (ATP), Eq. (3), measure the lethal concentration 50 (LC_{50}). Terrestrial toxicity potential (TTP), Eq. (4), measures the LD_{50} (Young and Cabezas, 1999).

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$$HTPI = \frac{1}{LD_{50}} \quad (1)$$

$$HTPE = \frac{1}{TLV} \quad (2)$$

$$ATP = \frac{1}{LC_{50}} \quad (3)$$

$$TTP = \frac{1}{LD_{50}} \quad (4)$$

Now, the atmospheric impacts are split into four categories: two global and two locals. Global warming potential (GWP), Eq. (5), measures carbon dioxide emission (a_{CO2}). Ozone depletion potential (ODP), Eq. (6), measures ozone concentration (O_3). Photochemical oxidation potential (PCOP), Eq. (7), evaluates the change in ethylene emission (a_{C2H4}). Acidification potential (AP), Eq. (8), determines the acidification potential for SO_2 (V_{SO2}) (Young and Cabezas, 1999).

$$GWP = \frac{\int_0^t a_i c_i(t)dt}{\int_0^t a_{CO_2} c_{CO_2}(t)dt} m_i \quad (5)$$

$$ODP = \frac{\delta[O_3]_i}{\delta\,[O_3]\,FCKW - 11} m_i \quad (6)$$

$$PCOP = \frac{\frac{a_i}{b_i(t)}}{\frac{a_{C_2H_4}}{b_{C_2H_4}(t)}} m_i \quad (7)$$

$$AP = \frac{\frac{V_i}{M_i}}{\frac{V_{SO_2}}{M_{SO_2}}} m_i \quad (8)$$

Where in Eq. (5) is the absorption of radiative heat per unit of greenhouse gas i, refers to this same absorption but per unit of carbon dioxide, is the concentration of greenhouse gas i at a time t after it has been released, refers to carbon dioxide, t is the number of years over which the GWP is to be evaluated, in Eq. (5) and Eq. (6) is the mass of the emitted gas, refers to the global ozone depletion produced by a unit of the gas i, is the ozone depletion produced by a CFC-11 unit, in Eq. (7) is the change in ozone concentration due to a change in the emission of a volatile organic compound i, refers to this same change, but concerning the emission of ethylene, is the integrated emission of a volatile organic compound i up to a time t, refers to this last condition concerning ethylene, in Eq. (7) is the mass of the volatile organic compound emitted, is the acidification potential of component i, is the acidification potential of SO_2, is the unit of mass of the substance i, is the unit of mass of SO_2 y in Eq. (8) is the mass of a significant component i emitted (Cabezas et al., 1999).

The WAR algorithm establishes a relationship between the potential environmental impact (PEI) and its transfer across system boundaries through the exchange of mass and energy, known as the PEI balance. To assess the environmental impact of a chemical process, it classifies indicators into two types: the emitted PEI, which measures the external environmental efficiency by reducing emissions, and the internally generated PEI, which reflects the environmental efficiency of the process. Both are expressed in terms of the unit of time and mass of the product, allowing to compare processes according to their potential environmental impact and generation rate. In addition, equations (9) to (12) are used to calculate the total output and generation rates of PEI, both in terms of impact and mass (Young and Cabezas, 1999).

$$i_{\text{out}}^{(t)} = i_{\text{out}}^{(cp)} + i_{\text{out}}^{(ep)} + i_{we}^{(cp)} + i_{we}^{(ep)} = \sum_{j}^{cp} M_j^{(out)} \sum_{k}^{cp} X_{kj}\psi_k + \sum_{j}^{ep-g} M_j^{(out)} \sum_{k}^{ep-g} X_{kj}\psi_k \tag{9}$$

$$\hat{l}_{\text{out}}^{(t)} = \frac{\left(i_{\text{out}}^{(cp)} + i_{\text{out}}^{(ep)} + i_{we}^{(cp)} + i_{we}^{(ep)}\right)}{\sum_P P_P} = \frac{\sum_j^{cp} M_j^{(out)} \sum_k^{cp} X_{kj}\psi_k + \sum_j^{ep-g} M_j^{(out)} \sum_k^{ep-g} X_{kj}\psi_k}{\sum_P P_P} \tag{10}$$

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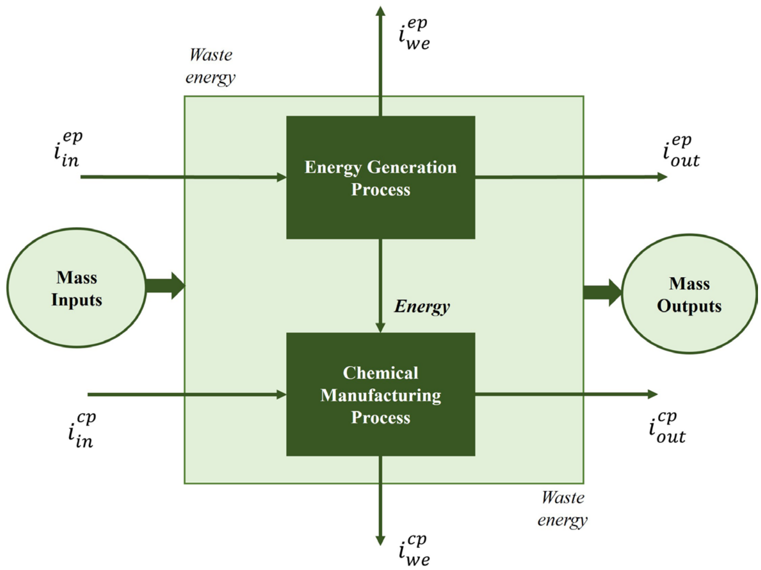
$$i_{\text{gen}}^{(t)} = i_{\text{out}}^{(cp)} - i_{\text{in}}^{(cp)} + i_{\text{out}}^{(ep)} - i_{\text{in}}^{(ep)} + i_{we}^{(cp)} + i_{we}^{(ep)} = \sum_{j}^{cp} M_j^{(out)} \sum_{k}^{cp} X_{kj}\psi_k - \sum_{j}^{cp} M_j^{(in)} \sum_{k}^{cp} X_{kj}\psi_k + \sum_{j}^{ep-g} M_j^{(out)} \sum_{k}^{ep-g} X_{kj}\psi_k \quad (11)$$

$$\hat{\imath}_{gen}^{(t)} = \frac{\left(i_{out}^{(cp)} - i_{in}^{(cp)} + i_{out}^{(ep)} - i_{in}^{(ep)} + i_{we}^{(cp)} + i_{we}^{(ep)}\right)}{\sum_P P_P} = \frac{\sum_j^{cp} M_j^{(out)} \sum_k^{cp} X_{kj}\psi_k - \sum_j^{cp} M_j^{(in)} \sum_k^{cp} X_{kj}\psi_k + \sum_j^{ep-g} M_j^{(out)} \sum_k^{ep-g} X_{kj}\psi_k}{\sum_P P_P} \quad (12)$$

Where $i^{(cp)}_{out}$ y $i^{(cp)}_{in}$ are the rates of entry and exit of PEIs from the system due to the chemical interactions that occur within the system, respectively; i^{ep}_{out} y i^{ep}_{in} are the speeds of entry and exit of PEIs of the system due to the energy generation processes in the system, respectively; i^{ep}_{we} y i^{cp}_{we} are the output impacts of the system as a result of the release of unused energy due to energy production and chemical processes occurring within the system, respectively; $M_j^{(in)}$ y $M_j^{(out)}$ are the mass flows of input and output of stream j, respectively; X_{kj} is the mass fraction of component k in stream j, Ψ_k is the overall Potential Environmental Impact of chemical substance k, and P_p is the mass flow of product p (Young et al., 2000).

Figure 2 shows the PEI balance, this approach considers a global balance, incorporating the material flows within the process (inputs and outputs) along with its energy consumption. To visualize the estimated total values and impact indicator categories, bar charts were generated for four scenarios. Case 1, serving as the baseline, considers only the impacts of waste, excluding energy resources and product flows. Case 2 accounts for the impacts of waste and product flow but omits energy contributions. Case 3 evaluates the impacts of waste and energy consumption. Case 4 encompasses the combined impacts of waste, energy consumption, and product flow. All four cases were used to construct the total impact chart, while only Case 4 was applied to analyze the individual atmospheric and toxicological categories. In addition, the hourly PEI production rate at different stages of the process was assessed, focusing only on waste and energy contributions, separately. Furthermore, impacts were quantified by category for energy flow and energy source using Case 3, providing a comprehensive assessment of environmental performance based on energy consumption.

Figure 2. *Potential environmental impact balance.*



3. Results and Discussion

Total potential environmental impact of mass and energy-integrated gas oil hydrocracking process

Figure 3 presents the total PEI generated and the total PEI produced per kilogram of product and per hour across all cases analyzed in the hydrocracking process. In Cases 1 and 3, the PEI generation rate is negative (−88,400 and −84,900 PEI/h, respectively), indicating that the process reduces environmental impacts by utilizing energy to transform a low-impact substance, such as gas oil fuel, into products with greater global impact potential. Conversely, Cases 2 and 4 show positive PEI generation rates over time (516,000 and 519,000 PEI/h, respectively), highlighting the substantial environmental impact of the process's products, which are classified as highly toxic substances with significant environmental implications.

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Figure 3. *Total potential environmental impact generated and output of mass and energy-integrated gas oil hydrocracking process.*

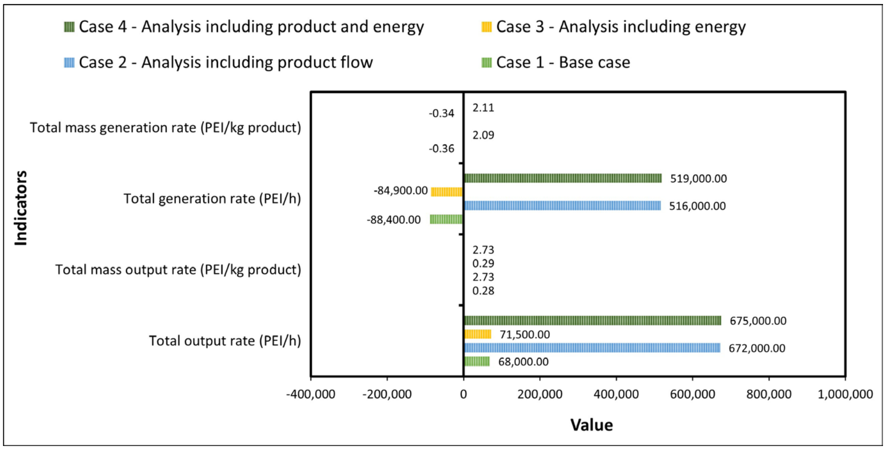

Figure 3 shows that Case 1 has the lowest output PEI at 68,000 PEI/h, as the process generates no hazardous substances in the waste streams, while Case 3 slightly increases to 71,500 PEI/h, indicating minimal contribution from energy to the output PEI. In contrast, Cases 2 and 4 display the highest values, 672,000 and 675,000 PEI/h, respectively, underscoring the significant environmental impact of the products, many of which are classified as hazardous by the EPA (Speight, 2011). Despite this, the PEI generation and production per kilogram of product were notably low due to the large amount of product generated (211,798 kg/h). Similar environmental evaluations in the literature in bioprocess, such as the biohydrogen production process from palm crop residual biomass, report much higher PEI production values, with 12,000,000 PEI/h in Case 4 (Gonzalez-Delgado et al., 2017), far exceeding the 675,000 PEI/h observed for the gas oil hydrocracking process in this study. On the other hand, in petrochemical industry processes, such as PVC production, a lower value of PEI produced was obtained in case 4 (5,890 PEI/day or 245 PEI/h) compared to the integrated mass and energy gas oil hydrocracking process; which may be because the products generated in this process (LPG, diesel, kerosene and naphtha) represent more polluting and harmful substances than PVC (González-Delgado et al., 2023).

Toxicological impacts of mass and energy-integrated gas oil hydrocracking process

Figure 4 illustrates the toxicological impact rates generated and produced in case 4 (waste, energy, and products) by the mass and energy-integrated gas oil hydrocracking process, focusing on human impacts (HTPI and HTPE) and environmental effects (ATP and TTP). The HTPI and TTP categories exhibit negative PEI generation rates (both of -16,800 PEI/h), indicating that the process converts raw materials such as gas oil fuel into products with greater impacts, including kerosene and diesel. On the other hand, the PEI rates for the HTPE and ATP categories are positive (66.2 PEI/h and 500,000 PEI/h, respectively), attributed to compounds like ammonia and hydrogen sulfide present in the waste streams.

Figure 4. *Toxicological impacts of mass and energy-integrated gas oil hydrocracking process.*

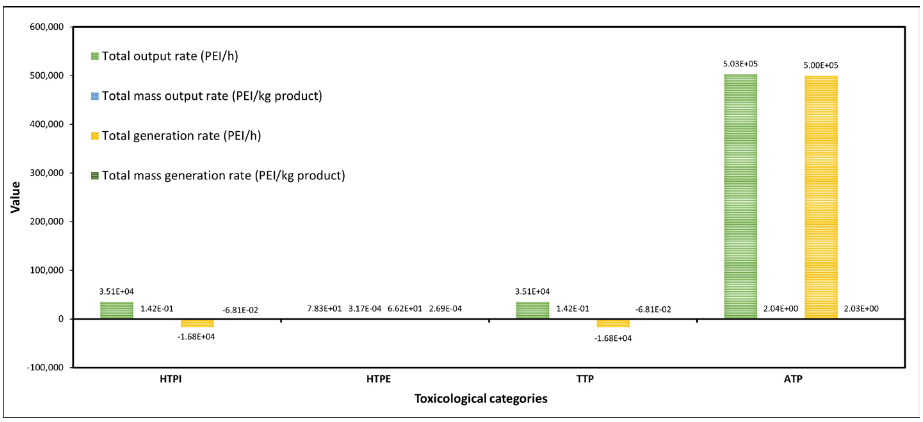

Figure 4 shows that the HTPI, TTP, and ATP categories have significant output impact values per unit of time, all of which are labeled. Notably, both the HTPI and TTP categories share a value of 35,100 PEI/h, primarily related to product streams. The HTPE category is mainly influenced by fuel, hydrogen, and sour gases, which are suspended in the air, resulting in an impact value of 78.3 PEI/h. In contrast, the ATP category has a much higher value of 503,000 PEI/h, reflecting the substantial presence of substances in the process that could potentially contaminate water bodies. The

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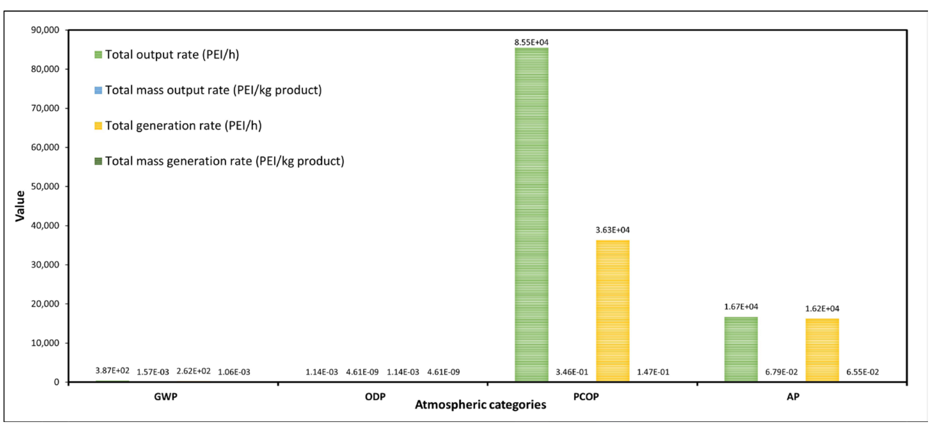
PEI generated per kilogram of product shows positive values for the HTPE and ATP categories and negative values for the HTPI and TTP categories. The output impacts per unit mass of the process product indicate that all categories have values below 2.5 PEI/kg.

Atmospheric impacts of mass and energy-integrated gas oil hydrocracking process

Figure 5 presents the atmospheric impact rates generated and produced in case 4 (waste, energy, and products) by the mass and energy-integrated gas oil hydrocracking process, focusing on global (GWP and ODP) and local (PCOP and AP) impacts. For the ODP category, both the generated and production values are below 1 PEI/h, as there are no significant contributions from substances released in waste streams or products, which are mainly liquid. The only gas streams exiting the process—combustion gases from the heaters, sour gases from the three-phase separators, and hydrogen from the PSA—mainly affect toxicological impacts. In contrast, the PCOP category showed the highest PEI values for both generation (36,300 PEI/h) and production (85,500 PEI/h) because the combustion gases, containing carbon oxides and methane, contribute to impacts in this category (Brough and Jouhara, 2020).

Figure 5. *Atmospheric impacts of mass and energy-integrated gas oil hydrocracking process.*

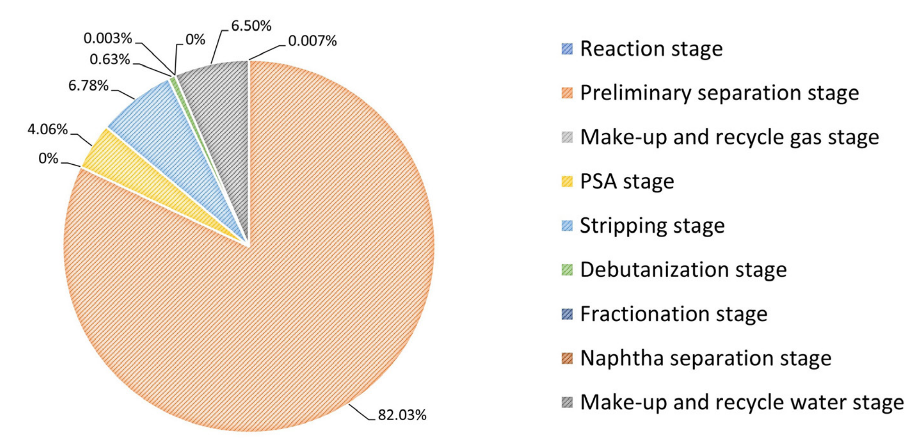


The AP category also recorded high PEI values (16,200 PEI/h generated and 16,700 PEI/h produced) due to chemical emissions in the vapor phase that contribute to acid rain potential. The GWP category, however, showed lower values (387 PEI/h output and 262 PEI/h generated), primarily from carbon oxides (CO_x) emitted during fossil fuel combustion in heaters. Despite these impacts, the PEI per kilogram of product for the five products generated—LPG, light and heavy naphtha, kerosene, and diesel—remained below 1 PEI/kg, indicating environmentally friendly production.

Contribution of process stages to total environmental impacts in the mass and energy-integrated gas oil hydrocracking process

Figure 6 presents an individual analysis of the stages of the integrated case of the gas oil hydrocracking process, taking into account the waste input. This analysis was carried out to understand the waste flows associated with each stage.

Figure 6. *Contribution of each stage of mass and energy-integrated gas oil hydrocracking process to the total PEI production rate considering waste*



According to Figure 6, the preliminary separation stage, which includes flash and three-phase separators, sour gas absorption towers, and heating and cooling services, produces a significant amount of PEI, contributing 82.03% (lower compared to the base case, 87.88%). This high value is linked to the waste streams from the

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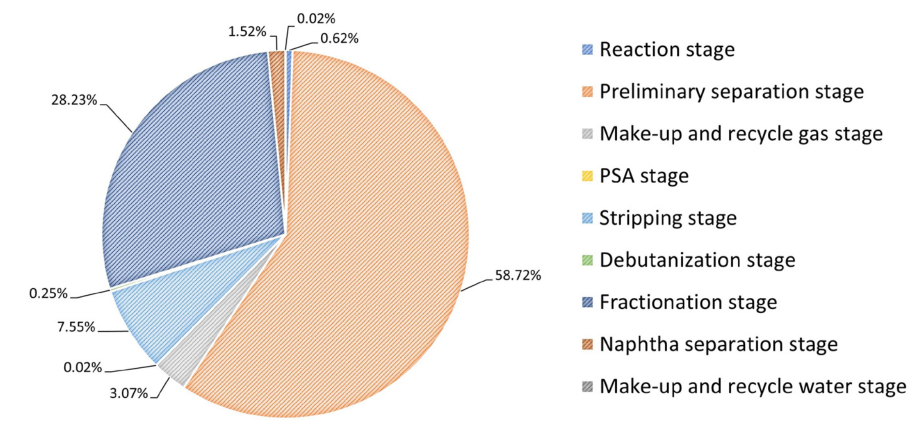
absorption towers (rich amine), which contain significant amounts of environmentally impacting substances such as ammonia and hydrogen sulfide. Next, the stripping, make-up and recycle water, and PSA stages contribute 6.78% (lower than the base case, 7.39%), 6.50%, and 4.06% (lower than the base case, 4.09%), respectively, while the debutanizer, reaction stage, and fractionator show much smaller contributions of 0.63% (same as the base case), 0.007% (lower than the base case, 0.008%), and 0.003% (same as the base case), respectively. Additionally, the naphtha separator stage does have waste streams (recycle water), but these are directed to the make-up and recycle water section, resulting in a contribution of 0%, as in the base case. Furthermore, the make-up and recycle gas stage do not produce any waste streams in the process, resulting in a contribution of 0%, as in the base case. It is worth noting that, in the integrated case, most of the contribution percentages decreased compared to the base case, due to the incorporation of a new stage in the process (make-up and recycle water stage) with significant residual effluents (wastewater).

Contribution of process stages to total environmental impacts in the mass and energy-integrated gas oil hydrocracking process via energy consumption

The values in Figure 6 change when only energy consumption is considered. Figure 7 illustrates the contribution of each stage to the total PEI of the integrated case of the gas oil hydrocracking process considering energy use.

Figure 7. *Contribution of each stage of mass and energy-integrated gas oil hydrocracking process to the total PEI production rate considering energy.*



According to Figure 7, the preliminary separation stage accounts for the largest share of total PEI production with 58.72% (higher than the base case, 51.86%), mainly due to its extensive equipment, resulting in higher energy consumption. Similarly, the fractionation stage contributes 28.23% of the total (lower than the base case, 32.86%), with the PEI coming from the energy used by the heater and the three distillation columns in series. In contrast, the stripping, and make-up and recycle gas stages, as well as the naphtha separator, contribute less to the PEI, at 7.55% (lower than the base case, 8.79%), 3.07% (lower than the base case, 3.57%), and 1.52% (lower than the base case, 1.77%), respectively, as they involve less energy-intensive equipment. In addition, the reaction, debutanization, make-up and recycle water, and PSA stages each contribute less than 1%, i.e., 0.62% (lower than the base case, 0.84%), 0.25% (lower than the base case, 0.29%), 0.02%, and 0.02% (lower than the base case, 0.03%), respectively. It should be noted that, in the integrated case, there was an increase in the energy requirements of the preliminary separation stage after carrying out the energy integration, due to this, the contribution percentage of this section increased, decreasing the others compared to the base case.

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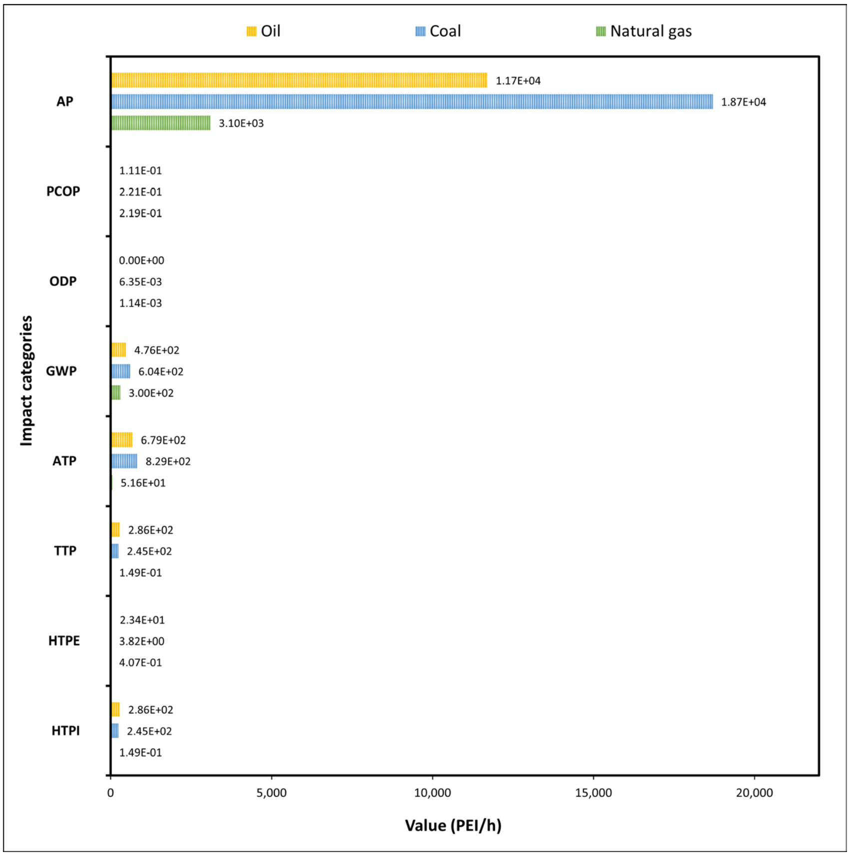
Potential environmental impact for atmospheric and toxicological categories of mass and energy-integrated gas oil hydrocracking process considering fuel type

Figure 8 illustrates the potential environmental impact (PEI) for both atmospheric and toxicological categories as a function of the fuel type used to meet the energy needs of the mass and energy-integrated gas oil hydrocracking process.

Figure 8. *PEI for atmospheric and toxicological categories of mass and energy-integrated gas oil hydrocracking process considering fuel type.*



This analysis focuses on Case 3, which accounts for the contributions from residues and energy used to produce the products. Among the eight categories, the acidification potential (AP) category is the most significantly affected by the energy consumption of the three fuel sources, recording values of 11,700 PEI/h for oil (higher than the base case, 10,100 PEI/h), 18,700 PEI/h for coal (higher than the base case, 16,100 PEI/h), and 2,670 PEI/h for gas (higher than the base case, 3,100 PEI/h). As expected, coal exhibits the highest environmental impact, with an acidification potential almost twice that of oil and almost nine times that of gas. Additionally, among other atmospheric impact categories, only global warming potential (GWP) shows significant values, measuring 476 PEI/h for oil (higher than the base case, 409 PEI/h), 604 PEI/h for coal (higher than the base case, 519 PEI/h), and 300 PEI/h for gas (higher than the base case, 257 PEI/h). In contrast, the photochemical oxidation potential (POCP) and ozone depletion potential (ODP) categories have much lower emission rates, each below 0.5 PEI/h, as in the base case.

According to Figure 8, the output potential environmental impacts (PEIs) for toxicological categories vary significantly depending on the energy source. The aquatic toxicity potential (ATP) category shows the most significant impacts, mainly due to the generation of ammonia and hydrogen sulfide, which tend to dissolve in water bodies. Other toxicological categories, such as terrestrial toxicity potential (TTP), human toxicity potential by inhalation (HTPE), and human toxicity potential by ingestion (HTPI), show slightly lower impacts, with HTPE recording the lowest impact. Figure 8 indicates that for the TTP, HTPE, and HTPI categories, oil is the energy source associated with the highest impacts, while coal leads in the ATP category. In this context, natural gas demonstrates superior performance in all categories, suggesting that it should be prioritized as the main energy source to meet process demands.

4. Conclusions

The Waste Reduction (WAR) algorithm was applied to evaluate the environmental performance of the mass and energy-integrated gas oil hydrocracking process on an industrial scale. This process converts raw materials with low potential environmental impact (PEI), like gas oil, into final products with higher PEI, such as LPG, heavy and light naphtha, kerosene, and diesel, resulting in increased PEI generation. The significant PEI production is mainly driven by the nature of the products, as seen in the positive total PEI values in Cases 2 and 4. The evaluation of toxicological impacts shows favorable performance, with only the HTPE and ATP categories exhibiting positive PEI generation values, the latter being the highest, while the HTPI and TTP categories showed negative values. Regarding atmospheric impacts, the PCOP and AP indicators recorded the highest values, directly related to pollutant emissions that contribute to smog and acid rain. Coal is the energy source that produces the most PEI in the atmospheric and toxicological categories. The preliminary separation stage is the one that contributes the most to the production of PEI, considering waste and energy separately. Overall, it can be concluded that the gas oil hydrocracking process is environmentally acceptable when compared to other biorefinery processes, such as biohydrogen production from palm biomass, which produces higher PEI/h values.

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