

Environmental Evaluation via Waste Reduction Algorithm (WAR) of an Energy-Integrated Suspension PVC Production Process

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The plastics industry has experienced exponential growth due to the versatility and low cost of its products. However, the high strength and durability of these materials have made them one of the main pollutants. This work focuses on the production of PVC (polyvinyl chloride), transforming vinyl chloride monomer (VCM), a highly polluting and hazardous raw material, into a material with lower environmental impacts. The main environmental problem of this industry is its high energy consumption, which generates significant emissions of toxic and greenhouse gases. An environmental assessment was carried out using the Waste Reduction Algorithm for a PVC production process with energy integration. In this analysis, the impacts of the output streams per unit of time and mass were calculated, also considering aspects such as energy consumption and product mass. This work provided a deeper understanding of the consumption of fossil fuels and natural gas, highlighting that the environmental impact of fossil fuels is up to eight times greater than that of natural gas. In addition, energy integration achieved a 9.8% reduction in the environmental impacts associated with energy consumption.

Keywords: PVC (Polyvinyl Chloride); Vinyl Chloride Monomer (VCM); Energy Consumption; Environmental Impact; Energy integration.

1. Introduction

Plastic is the material with the greatest boom in recent decades, being indispensable in our daily lives thanks to its flexibility and versatility to fulfill different functions, from the technological field to the manufacture of household utensils, despite all the benefits it can offer us; the mass production of this makes it a pollution problem due to its difficult degradation and sometimes recycling (Nishimura, 2018). PVC is one of the most widely used plastics globally (Čolnik et al., 2022). This is due to its low cost, high strength and low density, close to 1.4 g/cm³, in addition to its great versatility for various applications, thanks to additives that give it rigidity or flexibility as required. Another important quality is its stability and chemical inertness, which makes it suitable for sanitary products and drinking water pipes. Likewise, PVC stands out for its fireproof properties and its wide use as a material (Franco-Urquiza and Maspocho, 2014). Global development is aimed at the sustainability of industrial processes and at greatly reducing their environmental impacts (Del Carmen, n.d.), in order to increasingly conform to global objectives (United Nations, n.d.). carrying out environmental assessments to quantify the impacts produced or consumed by the processes gives us an outline of how sustainable they are (Moreno-Sader et al., 2021). There are different types of methodologies by which we can carry out this type of studies, this work analyzed an energy-integrated PVC production plant and has been carried out using the WAR GUI software, it is an accessible tool created by the United States Environmental Protection Agency (EPA) to analyze the environmental impacts associated with chemical processes. Its focus is limited exclusively to the manufacturing stage within the complete life cycle of a product, which significantly reduces the amount of information needed to perform the evaluation (Sammons et al., 2009).

To assess the possible environmental impacts, the WAR algorithm was used, which analyzes eight risk categories (Cassiani-Cassiani et al., 2018), Human toxicity by ingestion (HTPI), which assesses the danger of accidental or intentional ingestion of a substance, considering the lethal dose and long-term effects. ; Human

toxicity by dermal exposure or inhalation (HTPE), which quantifies the risks of contact of the substance with the skin or respiratory tract, analyzing irritation and other harmful effects; Aquatic Toxicity Potential (ATP), which measures the impact on aquatic organisms, from microorganisms to fish, considering their acute and chronic toxicity; Terrestrial toxicity potential (TTP), which assesses the effects on soil organisms, such as plants and microorganisms, and their ability to bioaccumulate; Global warming (GWP), which quantifies the substance's contribution to global warming in terms of its carbon dioxide equivalent; Ozone depletion (ODP), which measures the substance's ability to destroy the ozone layer, increasing exposure to ultraviolet radiation; Photochemical oxidation potential (PCOP), which assesses the substance's contribution to the formation of ground-level ozone and other photochemical oxidants harmful to health and the environment; and Acidification Potential (AP), which quantifies the substance's ability to acidify the environment, contributing to acid rain and acidification (Meramo et al., 2018).

2. Methodology

2.1 Process description

In Figure 1, the energy integrated industrial-scale suspension PVC production is described, the process begins with the introduction of VCM (vinyl chloride monomer) into the polymerization reactor, where it is mixed with a water suspension, a stabilizer (polyvinyl alcohol) and the polymer initiator (peroxide). The reaction occurs at 70 °C and 10 kgf/cm² pressure. The polymerization process occurs within the monomer droplets as the catalyst decomposes, and the reaction is exothermic with a typical conversion rate of 85%. After the reaction, a heterogeneous mixture remains, containing the suspended polymer, unreacted VCM, water, initiator and stabilizer, all at 3.5 kgf/cm² and 70 °C. To remove the unreacted monomer, the mixture undergoes a gasification step where the pressure is reduced to 1.8 kgf/cm², separating approximately 95% of the VCM. The remaining 5% is removed in a desorption column, which uses a high-pressure steam stream (14 kgf/cm²) at 225 °C to strip the monomer from the mixture. This process produces a monomer-rich upper stream and a lower stream with less than 1 ppm VCM.

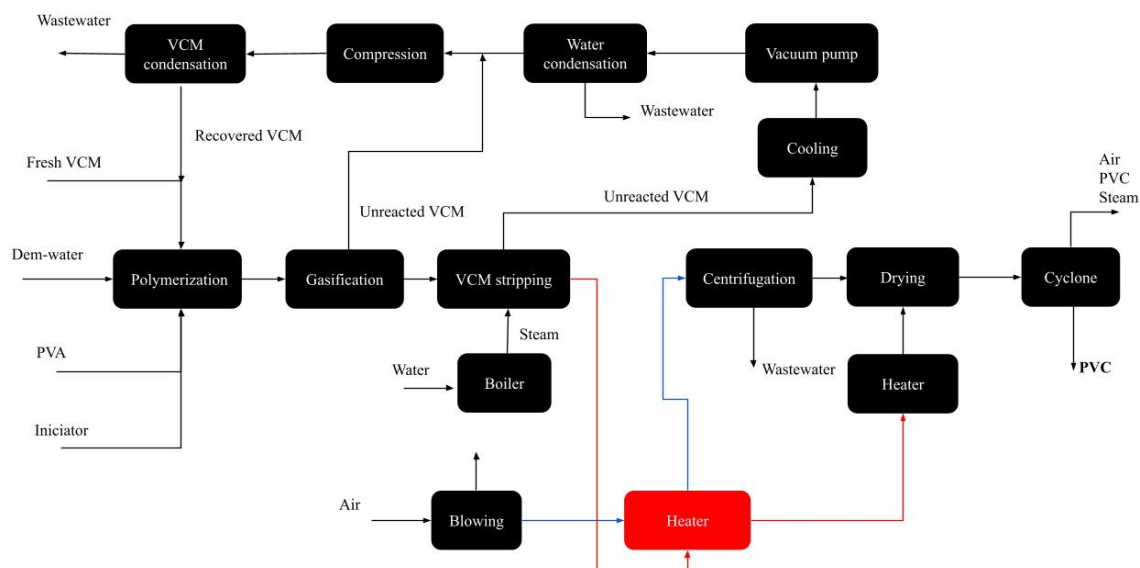


Figure 1: Energy-integrated suspension PVC production process diagram.

The monomer-rich stream is processed in a residual monomer recovery system that includes compressors and heat exchangers. This system prepares the VCM for recirculation by cooling the stream to 50 °C using a vacuum pump and condensing the VCM to separate it from the monomer. On the other hand, the stream coming from the bottom of the desorption column, composed mainly of water (approximately 70 %), is directed to a heat exchanger that extracts the excess heat, using it in a later stage of the process as part of the energy integration (Highlighted in red on the graph). Subsequently, this stream is sent to a centrifuge operating at 1,800 rpm,

removing 75 % of the water. The wastewater stream contains fractions of polymer, PVA and the initiator. The product stream leaving the centrifuge is a wet slurry, which is then dried using a stream of hot air at 250 °C to remove the remaining moisture. The drying process brings the temperature of the polymer blend to 70 °C, which reduces its moisture content. Finally, the dry polymer stream leaving the dryer is a gas mixture containing air, water vapor and polymer particles. This mixture passes through a cyclone where the dry polymer is separated from the residual gas mixture. The air and water vapor, containing 0.2% polymer, are separated through the upper stream, while the lower stream consists of the dry, granulated polymer with 0.01% moisture, which is ready for packaging and distribution.

2.2 Environmental assessment

In this work, the WAR algorithm and WAR GUI software were used to analyse the environmental impacts of the process, considering four cases: Case 1 excludes the contributions of energy and product; Case 2 includes the impact of the product in the PEI balance; Case 3 considers only energy sources; and Case 4 integrates all variables (process, product and energy). Three energy sources (gas, oil and coal) were evaluated, comparing their environmental performance. The analysis was carried out in eight impact categories: human toxicity by ingestion (HTPI), human toxicity by exposure (HTPE), aquatic toxicity (ATP), terrestrial toxicity (TTP), global warming (GWP), ozone depletion (ODP), photochemical ozone formation (PCOP) and acidification (AP) (Meramo-Hurtado et al., 2018), making it possible to evaluate the global and specific impacts per kilogram of product in each case.

3. Results and discussion

3.1 Total PEI: generation and output for energy-integrated suspension PVC production process.

Figure 2 shows that case 1 presents the best performance, with a net PEI output rate of -120,000 PEI/h, reflecting negative impacts attributable to the recycling of 99 % of the VCM and high energy efficiency. In contrast, the non-integrated system shows substantially higher values: in case 4, impacts reach 6340 PEI/day, due to high energy consumption and the inclusion of the product in the analysis (González-Delgado et al., 2023). Significantly higher PEI values per ton are also evident (3.02 and 5.5 PEI/ton in cases 3 and 4), while in the integrated system these remain close to zero. This comparison highlights how energy integration allows for an effective reduction of environmental impact, by optimizing energy use and recycling critical raw materials. However, in both integrated and non-integrated processes, product design and energy source are still decisive. It is recommended to complement energy integration with clean energy, sustainable PVC redesign and sensitivity analysis to mitigate key impacts.

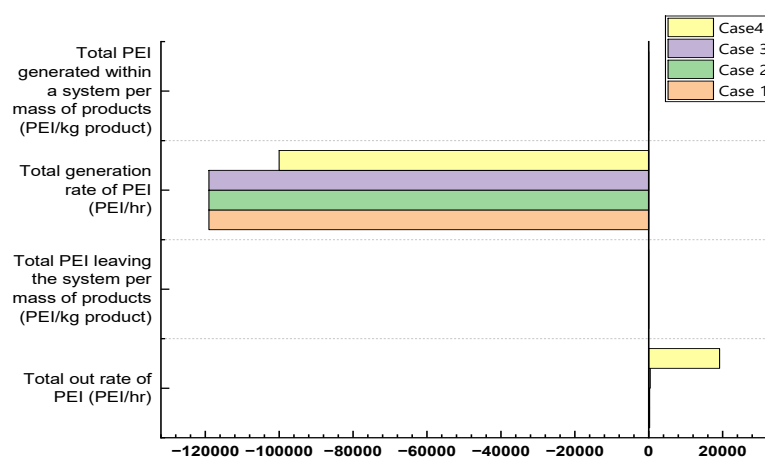


Figure 2. Total PEI output and generated in the energy-integrated suspension PVC production process.

3.2 Toxicological impacts: Generated and total mass output rates

From Figure 3, the energy-integrated PVC production process appears to reduce direct environmental impacts by converting a highly toxic raw material into a more benign product, as shown by lower HTPI and TTP values. However, in case 4, the presence of positive values in several impact categories suggests that energy integration may also introduce secondary environmental burdens—such as emissions from energy production or the use of non-renewable sources. A comparable situation is reported by Velásquez-Barrios et al., where the

photochemical oxidation potential (PCOP) in polypropylene production doubled from 138,000 to 276,000 when transitioning from 120 t to 240 t of transitional material, indicating how increased production or energy use can worsen certain indicators. These findings underscore the importance of evaluating energy integration comprehensively, considering not only process efficiency but also the sustainability of energy sources and the product lifecycle to truly minimize environmental impacts.

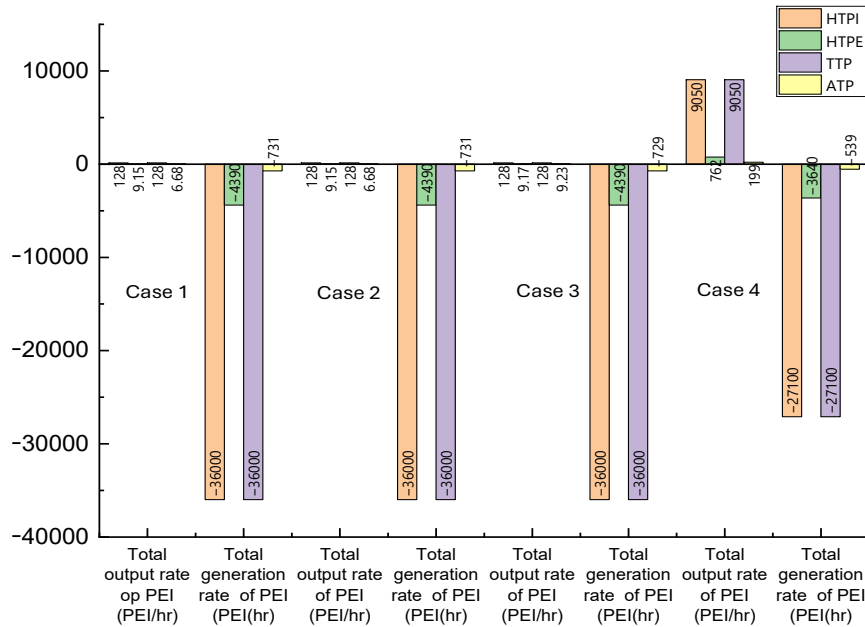


Figure 3. Toxicological impacts generated and local output of the energy-integrated PVC production process.

3.3 Atmospheric impacts: Generated and total mass output rates

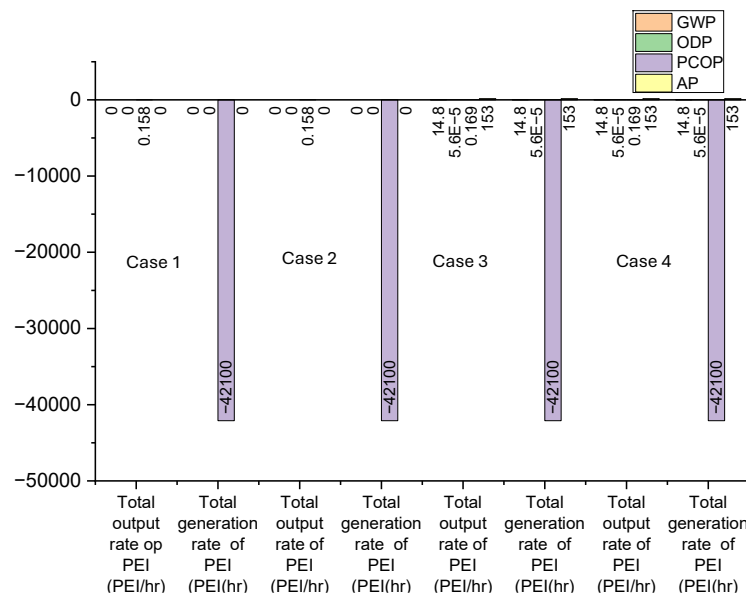


Figure 4. Atmospheric impacts generated and output from the energy-integrated PVC production process.

Figure 4 compiles the global (GWP and ODP) and local (PCOP and AP) atmospheric impacts corresponding to the energy-integrated suspension PVC production process. For global PEI values generated (14.8 and 0 PEI/h, respectively) and for local ones (-4210 and 0 PEI/h, respectively), denoting that in the GWP, ODP and AP categories a value of 0 PEI/h is recorded, which translates as a null contribution to the formation of substances

that affect the atmosphere. Furthermore, González-Delgado et al. (2023) recorded a GWP value of 510 PEI/day under normal process conditions, and for an energetically integrated case, a 30% reduction in atmospheric environmental impact was obtained with 355.2 PEI/day. On the other hand, the impacts associated with the Total output rate of PEI (PEI/h) where for the same atmospheric categories very low or null values are presented (0.0, 0.158 and 0, respectively) concluding that the PVC production process has an almost null contribution, however, like all industries, there are emissions, which are associated with the burning of fossil fuels. Although the PEI of each of the cases are not very high, there is a possibility that atmospheric impacts may increase, if and only if the raw material or the final product (PVC) come into contact with a heat source level, thus generating toxic or some carcinogenic vapors such as benzene, 1-butene, chlorobenzene, carbon monoxide, 1,3-butadiene, among others reported by Chong et al., (2019). González-Delgado et al. (2023).

3.4 Effect of energy sources

Figure 5 allows to compare the different contributions of three types of fuels, such as oil, natural gas and coal, from the perspective of each of the environmental impact categories relevant to the methodology in question, applied to the large-scale production process of energy-integrated PVC by suspension. Consequently, it is determined that energy sources such as oil or coal have excessively high impacts compared to natural gas, so much so that the burning of coal has a higher acidification impact (AP), contributing 923 PEI/h. In other words, natural gas has a better environmental performance as an energy source for the PVC production process.

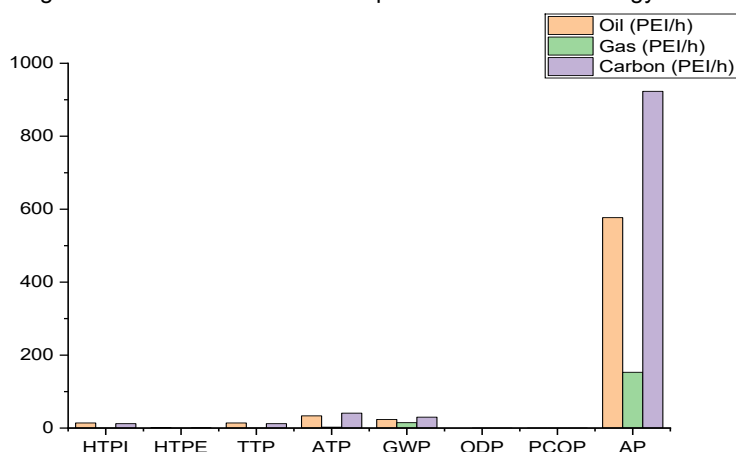


Figure 5. Environmental impacts depending on the energy source for the energy-integrated PVC production process.

4. Conclusions

Energy integration in PVC production represents a key strategy to improve the environmental sustainability of the process. The production process significantly reduces the toxicity of raw materials by transforming them into safer products, which is reflected in lower human toxicity (HTPI) and terrestrial toxicity (TTP) with a total output rate of 128 PEI/h for each category. It also contributes to minimizing atmospheric impacts, such as global warming (GWP) and ozone layer depletion or ODP (0.000056 PEI/h), through a more efficient use of energy resources. The use of natural gas as the main source maximizes these benefits, as it presents the lowest environmental impacts in all the metrics evaluated, contrasting with oil and coal, which generate high impacts in acidification or AP (153 PEI/h) and GWP (14.8 PEI/h). However, it is important to consider possible secondary effects, such as additional emissions under certain conditions, which could result from energy integration. Therefore, it is recommended to optimize operating conditions, prioritize cleaner energy sources and develop a sustainable PVC design that considers recyclable materials and a lower impact in its life cycle, thus ensuring a comprehensive reduction of environmental impacts in the process.

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Nomenclature

HTPI - Human Toxicity Potential by Ingestion.
 HTPE - Potential human toxicity by inhalation or dermal exposure.
 ODP - Ozone Depletion Potential.
 GWP - Global Warming Potential.
 PCOP - Potential Photochemical Oxidation Potential.
 AP - Acidification potential.
 ATP - Aquatic Toxicity Potential
 TTP - Terrestrial Toxicity Potential.
 PEI - Potential Environmental Impact

References

- Cassiani-Cassiani, D., Meza-González, D. A., & González-Delgado, Á. D. (2018). Environmental evaluation of agar production from macroalgae *Gracilaria* sp. *Chemical Engineering Transactions*, 70, 2005–2010. doi.org/10.3303/CET1870335
- Chong, N. S., Abdulramoni, S., Patterson, D., & Brown, H. (2019). Releases of Fire-Derived Contaminants from Polymer Pipes Made of Polyvinyl Chloride. *Toxics*, 7(4), 57. doi.org/10.3390/toxics7040057.
- Čolnik, M., Kotnik, P., Knez, Ž., & Škerget, M. (2022). Degradation of Polyvinyl Chloride (PVC) Waste with Supercritical Water. *Processes*, 10(10), 1940. doi.org/10.3390/pr10101940
- Del Carmen, D. S. M. (s. f.). *Green Chemistry: A New Approach to Environmental Care*. www.scielo.org.mx/scielo.php?script=sci_arttext&pid=S0187-893X2009000400004 (in Spanish)
- Franco-Urquiza, E., & Maspoch, M. L. (2014). Feasibility of reusing PVC waste from electrical cables: mechanical properties. *Afinidad*, 71(567). (in spanish)
- González-Delgado, Á. D., Ramos-Olmos, M., & Aguilar-Vásquez, E. (2023). Environmental Impacts Assessment in Suspension PVC Production Process Using Computer-Aided Process Engineering. *Polymers*, 15(13), 2902. doi.org/10.3390/polym15132902
- Marson, A., Manzardo, A., Piron, M., Fedele, A., & Scipioni, A. (2021). Life cycle assessment of PVC - A polymer alloy pipes for the impacts reduction in the construction sector. *Chemical Engineering Transactions*, 86, 721–726. doi.org/10.3303/CET2186121
- Meramo, S. I., Bonfante, H., De Avila-Montiel, G., Herrera Barros, A., & González-Delgado, A. (2018). Environmental assessment of large-scale production of TiO₂ nanoparticles using green chemistry. *Chemical Engineering Transactions*, 70, 121. doi.org/10.3303/CET1870203. (In Spanish)
- Meramo-Hurtado, S., Ojeda-Delgado, K., & Sanchez-Tuiran, E. (2018). Environmental assessment of a biorefinery: case study of a purification stage in biomass gasification. *Contemporary Engineering Sciences*, 11(3), 113-120. doi.org/10.12988/ces.2018.813
- Moreno-Sader, K. A., Martínez-Consuegra, J., & González-Delgado, Á. D. (2021). An integrated biorefinery approach via material recycle/reuse networks for the extraction of value-added components from shrimp: Computer-aided simulation and environmental assessment. *Food And Bioproducts Processing*, 127, 443-453. doi.org/10.1016/j.fbp.2021.04.003
- Nishimura, I. (2018). Strategy for Plastics in a Circular Economy. *Seikei-Kakou*, 30(11), 577-580. doi.org/10.4325/seikeikakou.30.577
- Sammons, N., Yuan, W., Bommareddy, S., Eden, M. R., Aksoy, B., & Cullinan, H. (2009). A Systematic Framework to Calculate Economic Value and Environmental Impact of Biorefining Technology. *En Computer-aided chemical engineering/Computer aided chemical engineering* (pp. 2007-2012). doi.org/10.1016/s1570-7946(09)70725-4
- United Nations. (n.d.). Sustainable Development Goals | United Nations. www.un.org/es/impacto-acad%C3%A9mico/page/objetivos-de-desarrollo-sostenible (in spanish)
- Velásquez-Barríos, A., Rueda-Duran, C., Mogollón, E., Alvarez, JC, Cardona, R., & Cardona-Alzate, CA Environmental impact analysis using the WAR Waste Reduction Algorithm in the polypropylene production process by applying grade transition strategies. (in Spanish)