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Process Design and Carbon Footprint Analysis of the Isopropanol Solvent Extraction of Petroleum Nut Oil

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ABSTRACT

The potential of petroleum nut (*Pittosporum resiniferum*) oil (PNO) as a raw material for biodiesel and a source of valuable compounds demands the investigation of its large-scale extraction. Previous laboratory extraction experiments of PNO were already conducted. This study investigates the scale-up of the laboratory process. DWSIM, a free chemical process simulation software, was used to generate a process model for PNO solvent extraction with a capacity of 8,881 kg/day. The Hansen solubility parameters were applied. The generated process model had comparable oil recovery to other solvent extractions. Using the process data from DWSIM, the carbon footprint intensity method was applied to estimate the carbon footprint of the extraction process and determine hotspots for carbon footprint reduction. The theoretical oil yield from the simulation is 33.73%, based on theoretical solubility interactions. The total cost and carbon footprint of the process are USD 1.03 M and 143 tCO_2/day. The cost is high because the current price of petroleum nut is for small-scale production. The overall carbon footprint can be reduced by 3.60% if the de-oiled cake were turned into briquettes and used as fuel to generate steam. This study contributes to alternative renewable energy sources as well as carbon footprint reduction analysis for process industries.

KEYWORDS

Process design, Pittosporum resiniferum, Solvent extraction, DWSIM, Carbon footprint intensity method, Simulation, Renewable energy

INTRODUCTION

Petroleum nut, *Pittosporum resiniferum*, oil (PNO) has shown great potential as a biodiesel raw material and a source of high-value products in the food and pharmaceutical industries. The potential of petroleum nut as a biodiesel raw material was investigated [1]. The petroleum nut biodiesel was found to exhibit similar properties to petroleum diesel [2]. PNO contains terpenes, such as myrcene and alpha-pinene [3], which are relevant materials in the food and pharmaceutical industries [4]. A critical part in the production of PNO is the extraction of oil from the nut.

Some of the techniques used in the extraction of nut oils are distillation, mechanical expression, solvent extraction, and supercritical fluid extraction. Earlier studies investigated the physicochemical characteristics of petroleum nut oil after steam distillation [5]. Other studies investigated the various volatile components of oil after steam distillation [6]. In a recent study, Soxhlet extraction was preferred over steam distillation in the extraction of oil from cashew nut shells since there was more oil extracted in mass per volume [7]. There was only a slight difference in the amount of extracted oil; hence, steam distillation is still a relevant extraction method.

Another conventional technique to extract nut oils is via mechanical pressing. Two extraction methods through mechanical means, hydraulic, and screw pressing were investigated [8]. Both methods utilize the same principle for the extraction of nut oils. However, the extraction using the hydraulic method applies extreme pressure, up to 100 MPa, via vertical compression of nuts. On the other hand, extraction is carried out at ambient temperature for screw pressing to recover high-quality oils [8]. A summary of several studies that adapted mechanical screw-pressing to extract nut oils from different nuts (almond, pistachio, and walnut) in a pilot plant and on an industrial scale was also discussed [8]. The use of screw pressing resulted in high oil recoveries (g extracted oil / g oil present), 79.3 % for almond; 79.6 % for pistachio, and 89.3 % for walnut. On the other hand, hydraulic pressing, specifically cold pressing, can lead to high oil yields, up to 82.34 % [9]. This yield was obtained by increasing the applied pressure and pressing times in the extraction of tiger nut (*Cyperus esculentus* L.) oil. Hence, both hydraulic pressing and screw pressing can produce high extraction yields of nut oils.

The extraction of nut oils via mechanical pressing seems promising because of high oil recoveries. However, it might not be the case for other nut oils. Another technique to extract nut oils is via solvent extraction. Leaching, also known as solid-liquid extraction, is the principle behind solvent extraction of a soluble component (either solid or liquid) from an insoluble solid using a solvent that is only miscible with the former material [10]. In a review of extraction technologies for tiger nut (*Cyperus esculentus* L.) oil [11], the solvent extraction method was commonly utilized in the extraction of oil content from oilseeds due to its high extraction rate compared with mechanical expression methods. A study conducted on tiger nut oil yielded 41.2 % (g oil extracted/ g of ground tiger nut) using the solvent extraction method with n-hexane [12]. In a similar experiment, the extraction of tiger nut oil via solvent extraction obtained a yield of 21.92 % (g oil extracted/ g of ground tiger nut) using a solvent mixture of chloroform and methanol (2:1, volume/volume) [13]. This yield is relatively small compared with the previous study due to the nature of the solvent. In the extraction of petroleum nut oil, a variety of organic solvents, namely hexane, ethanol, isopropanol, and cyclohexane, were investigated [14]. Among the solvents, using ethanol produced the highest oil yield, about 15.38 % (g oil extracted/ g of petroleum nut), followed by isopropanol, cyclohexane, and hexane with 14.74 %, 13.93 %, and 11.67 %, respectively [14].

A laboratory-scale extraction of petroleum nut oil was already conducted, which is a critical reference for its scale-up. Parametric and optimization studies about the extraction of petroleum nut oil via the solvent extraction method were conducted [14]. The effects of soaking time, solvent-to-nut ratio, and temperature in using various solvents, such as ethanol, isopropanol, hexane, and cyclohexane, in extracting the nut oil were determined [14]. Ethanol was found to be the most effective solvent with an oil yield and oil recovery of about 15.38 % and 43.92 %, respectively, at an extraction temperature of 50 °C, ethanol to nut ratio of 3.5 mL/g, and soaking time of 12 h [14]. The research implies the potential of a larger-scale solvent extraction of petroleum nut oil. In this study, however, isopropanol is investigated instead of ethanol. Isopropanol has the second-highest oil yield with 14.74% [14]. While ethanol showed a marginal advantage in yield under controlled laboratory conditions, isopropanol offers superior physicochemical characteristics for industrial applications where moisture control is variable **[15].** Isopropanol is less polar than ethanol, indicated by a lower dielectric constant, which increases its affinity for non-polar oil components. The longer, more hydrophobic carbon chain of isopropanol allows it to interact with non-polar groups in triglycerides and other lipids (which are present in Petroleum nut oil) compared to ethanol. These properties, combined with a lower unit price compared to ethanol, suggest that isopropanol provides a more comprehensive economic benefit for large-scale production.

Solubility parameters quantitatively describe the "like dissolves like" interaction among compounds. It predicts the miscibility among liquids such that similar solubility parameters generate good miscibility. The concept of Hildebrand solubility parameters was proposed [16]. The Hildebrand solubility parameter refers to the square root of the cohesive energy density. The Hildebrand solubility parameter was modified to consider the total heat of vaporization into dispersion, dipole, and hydrogen bonding forces [17], noting that these forces contribute to the total heat of vaporization. Hence, Hansen solubility parameters are in terms of the individual forces, which can be accessed from literature [17]. Solubility models were developed to predict the solubilities of compounds. One of which is the Flory-Huggins model [18]. It is a mathematical model that predicts the retention factor, which refers to the ratio of the solute concentrations in the non-polar (solid) and polar (solvent) phases, respectively [18]. The Flory-Huggins model in the extraction of rosmarinic acid from *Orthosiphon aristatus* [18]. Results show that the model generated a comparable recovery with experimental data using Hansen solubility parameters. Hence, the Flory-Huggins model is a good predictive model of solubility.

Aside from high product yield and lower operational costs, environmental metrics are now as important. Carbon footprint is of interest because of its direct impact on climate change. "Hotspots" or opportunities for carbon footprint reduction are determined using tools like Life Cycle Assessment. A growing approach to carbon footprint assessment has been gaining attention for more than a decade since its development. An interesting application of pinch analysis to address increasing CO_2 emissions was proposed [19]. The study developed a methodology that estimates the minimum amount of zero-carbon energy resources (biomass, wind, water, etc.) needed to comply with the energy demand and CO_2 emission limits of energy sectors [19]. This strategy utilizes a graphical approach wherein the Pinch analysis technique was adapted to determine the required zero-carbon energy resource for energy planning purposes [19]. The method is called carbon emission pinch analysis (CEPA).

The CEPA technique was adapted by another study to explore its application for chemical processes [20]. In the study, a special case of CEPA was developed, which is a new technique for carbon footprint reduction. It was called the carbon footprint intensity method [20]. From the adaptation of CEPA, carbon footprint composite curves are also used for analysis. Since the innovative method focuses more on CO_2 emission from chemical processes, the structure of the composite curves, which were the demand and supply curves, was quite different from CEPA. In chemical processes, both material and energy are inputs and outputs of the system; hence, both have their respective carbon footprints. As a result, material-based and energy-based emissions are considered in the analysis via the carbon footprint intensity method [19]. Energy-based emissions can be further disaggregated into internal and external emissions for in-depth analysis [20]. Composite curves are also generated in an innovative method, but they are plotted in a different manner. The demand composite curve is generated from a CO_2 emission benchmark, which is based on industry standards, competitive demands, or company decisions, as the dependent variable, while its corresponding economic value is the independent variable [20]. On the other hand, the source/supply composite curve is generated from the component emissions (material-based and energy-based or internal and external emissions) as the dependent variable, while its economic value is the independent variable. The curves or lines are also plotted with respect to increasing slope, like in CEPA. However, in the carbon footprint intensity method, the slope is referred to as carbon intensity, which is the ratio of CO2 emission and economic value [20]. Once the plots are generated, the pinch point is determined in a similar manner with respect to CEPA. Then, necessary analyses can be conducted for carbon footprint reduction.

A large-scale production of petroleum nut oil may have the potential to be a renewable energy source. However, there is a lack of information between the small-scale and large-scale extraction processes. Therefore, this research investigates the carbon intensity of a PNO solvent extraction plant through process modelling and the carbon footprint intensity method. This research utilizes DWSIM, a free chemical process simulation software, to generate the process model and conduct material and energy balances of a PNO solvent extraction plant. The necessary data for carbon footprint analysis were generated using the simulation software. To assess the carbon footprint of the proposed extraction plant, the carbon footprint intensity method [20] was used. This study serves as a foundation for the implementation of a pilot-scale solvent extraction of petroleum nut oil and other related studies. It provides a picture of the carbon footprint and carbon intensity of the extraction process and identifies a hotspot for carbon footprint reduction. It is important to note that this research is based on process simulation using theoretical modeling and literature data. Thus, the absence of experimental pilot-scale validation is a limitation of this study. Nevertheless, these results provide the essential theoretical framework and techno-economic and carbon footprint baseline required to justify and design future pilot-scale studies.

METHODOLOGY

Process modeling using DWSIM

This study adopted the parameters from the batch solvent extraction of petroleum nut oil by [14] using isopropanol as a solvent as the basis for the pilot-scale model. DWSIM was used to design the solvent extraction model. The simulation process model includes the extraction, solvent recovery, and water removal stages, respectively. Also, the packaging of the extracted oil in drums was not included. No pilot-scale or industrial solvent extraction plants of petroleum nut oil were found as a reference. Thus, this study adopted the process of avocado oil extraction from a simulation study [21] and integrated it with the experimental petroleum nut oil extraction [14]. DWSIM offers a wide range of compounds that can be used to model any material. Dried petroleum nut and petroleum nut oil were modelled in terms of their components. The compositions of both were calculated based on literature values. Table 1 shows the calculated composition of dried petroleum nut.

Table 1. Composition of dried petroleum nut

Component	Mass fraction [%]
Moisture	55.8800
Solid	9.6642
Linoleic acid	12.5281
Myrcene	11.245
Alpha-pinene	10.6827

The extraction of petroleum nut oil in terms of its components was modelled using Hansen solubility parameters and the Flory-Huggins model (Eq.1). This approach was used by a previous study to model the extraction of rosmarinic acid from *Orthosiphon aristatus*, which generated comparable oil recoveries to experimental runs [18].

$$ln\, k_s = \frac{v_i}{RT}[(\delta_i - \delta_m)^2 - (\delta_i - \delta_s)^2] \quad (1)$$

Where: k_s is the retention factor, v_i is the molar volume, R is the gas constant, δ_i is the solubility parameter of solute, δ_m is the solubility parameter of solvent, and δ_s is the solubility parameter of solid. Raoult's Law was the thermodynamic property package used in the process model. The extraction parameters, such as temperature, soaking time, and solvent-to-nut ratio (mL solvent per g dried nut), used were based on the conditions of the previous study [14]. The extraction temperature, soaking time, and solvent-to-nut ratio were 50 °C, 12 h, and 3.5 mL/g, respectively [14].

To estimate the carbon footprint of the process, a hypothetical solvent extraction plant was established. The designed production capacity of the extraction plant was 8,880.90 kg/day of PNO, which was calculated based on the current production capacity of a commercial biodiesel (coco methyl ester) plant in the Philippines. From the amount of biodiesel produced, the amount of PNO (raw material) was back calculated using the PNO biodiesel yield (g biodiesel produced per g PNO) based on the procedure of a study [2]. The required amount of dried petroleum nuts was calculated using an initial oil yield from an initial simulation run of the process, wherein 100 kg/day of dried petroleum nuts was used as a basis. Eq.2 was used to determine the required dried petroleum nut to produce 9,406.57 kg/day PNO.

$$Amount\ of\ Dried\ \ Petroleum\ Nut = \frac{Extracted\ PNO}{Oil\ Yield} \tag{2}$$

The amount of fresh petroleum nuts was estimated based on the pretreatment of jatropha. Table 2 shows established conversion factors for Jatropha pretreatment, which were used to predict the amount of fresh petroleum nuts needed. The fresh nuts were calculated from the dried nuts to the dirty fresh nuts using the conversion factors. Note that in PNO extraction, the seeds were removed, while the fruit pulp and husks were used for extraction.

Table 2. Pretreatment conversion factors

Pretreatment Process	Conversion Factor	Comment
Cleaning	0.95	kg clean fruit per kg dirty fruit
Husking	0.75	75 % of a nut is fruit pulp and husk
Drying	0.66	kg dried nuts per kg fresh nuts

The heat released or absorbed was calculated by DWSIM. In the first heat exchanger of the process (Heat Exchanger 1), the required heating water was manually calculated using the heat calculated by DWSIM. The initial and final temperatures of heating water were assumed to be 75 °C and 60 °C, respectively. In distillation operations (solvent recovery and water removal), the distribution of compounds in the distillate and bottoms streams was determined using DWSIM based on the distillation settings. The necessary inputs in distillation in DWSIM were the mole fractions of the light key (LK) and heavy key (HK) components in the bottoms and distillate streams, respectively. The LK component was chosen as the compound that would evaporate first. On the other hand, the compound that would evaporate next was the HK component. In the solvent recovery operation, LK and HK components were isopropanol and water, respectively. The input mole fraction of LK (isopropanol) in the bottoms stream was 0.0001 to ensure that most of it would go to the distillate stream. The input mole fraction of HK (water) in the distillate stream was 0.00001 to ensure that isopropanol would be concentrated in the distillate stream. In the water removal operation, LK and HK components were water and alpha-pinene, respectively. The input mole fraction of LK (water) in the bottoms stream was 0.0045 to ensure moisture was at most 0.05 % in the bottoms stream, since the required moisture for biodiesel is at most 0.05 %. On the other hand, the input mole fraction of HK (alpha-pinene) in the distillate stream was 0.001 to ensure that alpha-pinene would go to the bottoms stream. The Flory-Huggins model was used to simulate the extraction of PNO. It was applied using the spreadsheet tab of DWSIM, which can import values from the flowsheet and export values from the spreadsheet. Hence, the retention factors were calculated using the Flory-Huggins model (Eq.1) in the spreadsheet tab. The Hansen solubility parameters were calculated using Eq.3. The total parameter was used in the Flory-Huggins model. The total solubility parameter of the solid component was 25 $MPa^{0.5}$, which was based on the solubility parameter of lignin [22].

$$\delta_t = \sqrt{\delta_d + \delta_p + \delta_h} \tag{3}$$

Where: δ_t is the total solubility parameter, δ_d is the dispersion parameter, δ_p is the polar parameter, δ_h is the hydrogen bonding parameter. Table 3 shows the Hansen solubility parameters [17]. Eq.4 was used to calculate the amount of solutes (isopropanol, water, linoleic acid, myrcene, and alpha-pinene) that remain in the solid phase. Note that the retention factor refers to the ratio of solute concentration in the solid and solvent phases, respectively.

Table 3. Hansen solubility parameters [$MPa^{0.5}$] [17]

Compound	δ_d	δ_p	δ_h
Isopropanol	15.80	6.10	16.4
Linoleic Acid	18.29	2.94	7.24
Myrcene	16.00	1.60	2.20
Alpha-pinene	16.90	1.80	3.10
Water	15.50	16.00	42.30

$$k_s = \frac{\frac{x}{A}}{\frac{B - x}{C}} \tag{4}$$

Where: x is the amount of solute in solid phase, A is the amount of solid, B is the amount of solute, and C is the amount of solvent in solvent phase. After the amount of solutes in the solid and solvent phases were calculated, the separation factor of each solute was calculated using Eq.5. The separation factor was defined as the fraction of solute that goes to the miscella (solvent phase).

$$Separation\ factor = \frac{Amount\ of\ solute\ in\ solvent\ phase}{Amount\ of\ solute} \tag{5}$$

The calculated separation factors were then exported to the compound separator (CS-1) on the flowsheet tab of DWSIM. To explain the distribution of compounds in the solvent phase, the solubility parameter distance (Ra) between the solvent and solutes was calculated using Eq.6, where subscripts 1 and 2 refer to solute and solvent, respectively.

$$R_a = \sqrt{4(\delta_{d1} - \delta_{d2})^2 + \left(\delta_{p1} - \delta_{p2}\right)^2 + (\delta_{h1} - \delta_{h2})^2} \tag{6}$$

Carbon footprint analysis

In carbon footprint analysis, the scope of analysis is important. In this study, only the extraction process was considered, which starts with the mixing of dried petroleum nuts and isopropanol and ends with water removal in the extracted PNO. The carbon footprint of pretreatment was also considered, but it was considered as the carbon footprint of the dried petroleum nut. The downstream packaging of the extracted oil was excluded from the system boundary. This exclusion is justified because the extracted PNO is produced as an intermediate feedstock for further downstream processing. For example, transesterification for biodiesel production or fractionation for pharmaceutical applications. Therefore, packaging emissions were viewed outside the scope of the analysis. The material component refers to the materials used in the extraction process. The materials used were petroleum nuts and isopropanol. Water for heating and cooling purposes was not considered as part of this component since it was not directly involved in the extraction process. Water was considered a utility; hence, it was considered part of the energy-based component. The consumption of the material-based component was determined from the material balance. The unit cost of petroleum nuts was based on personal communication with the supplier. On the other hand, the unit cost for isopropanol was obtained from literature. The unit cost of petroleum nut is 16.94 USD/kg, while the unit cost of isopropanol is 0.85 USD/kg. Note that the cost of petroleum nut is relatively high because the production is small-scale in the Philippines.

The energy component refers to the utility (water and steam) and energy consumption of the extraction process. It was further classified into internal and external components. The internal component refers to steam generation and cooling water usage since both generate carbon footprint within the extraction facility. On the other hand, the external component refers to electricity and diesel consumption since both generate carbon footprint beyond the extraction facility. The diesel was used as fuel for the water heater to produce hot water. The amounts of heating water, superheated steam, and cooling water were calculated from the material and energy balance. The amount of diesel used was determined based on the required amount of heating water. Electricity consumption of the extraction process was based on the electricity requirements of the agitator and centrifuge only. The costs of the components were obtained from the literature. Table 4 shows the unit costs of energy components in 2025 in the Philippines. The conversion factor is USD 1 is to PHP 59.01.

Table 4. Costs of energy components in 2025 in the Philippines

Component	Cost [USD/unit]
Steam [kg]	0.014
Cooling water [kg]	0.00092
Electricity [kWh]	0.20
Diesel [kg]	1.08

The material-based footprints were determined using emission factors obtained from the literature. The emission factor used for petroleum nuts was based on the emission factor of jatropha in biodiesel production, which is 46.18 kg CO_2/kg nut-year [23]. The emission factor was based on the plantation, pretreatment, and hauling (from the plantation to the facility) of jatropha. It was assumed that the same conditions apply to petroleum nuts. On the other hand, the emission factor for isopropanol was based on the CO_2 emission per kilogram of isopropanol produced, which is 1.63 kg CO_2/kg isopropanol [24]. Similarly, the energy-based footprints were determined using emission factors obtained from the literature. The emission factor for steam was based on the heat released by steam in kWh. The emission factors for cooling water, electricity, and diesel were based on their respective consumptions. Table 5 shows the emission factors used for energy-based footprints.

Table 5. Energy-based emission factors

Component	Emission Factor [kg CO_2/unit]	Reference
Steam [kWh]	0.2264	[25]
Cooling water [m^3]	0.3760	[26]
Electricity [kWh]	0.7600	[27]
Diesel [kg]	3.1670	[28]

The carbon footprint intensity analysis of Tong kat Ali extract pilot plant was adopted for the petroleum nut oil solvent extraction plant [20]. First, material-based and energy-based composite curves were generated. To generate the source composite curves, the amounts of CO_2 emitted by utilized material and energy components were determined using the data generated from the simulation and emission factors from the literature. To generate the material-based composite curve, the total material cost and carbon footprint were obtained and plotted as x- and y-values, respectively, from the origin. To plot the energy-based composite curve, the total energy component cost and carbon footprint were obtained and plotted as x- and y-values, respectively, from the terminal point of the material-based composite curve, not from the origin. It can be observed that the material-based segment was plotted before the energy-based segment. In generating the source composite curve, the segments are plotted with increasing slope (carbon intensity). It was initially assumed that the material-based segment was less steep (less carbon-intensive) than the energy-based segment because the latter is usually more carbon-intensive than the former.

As for the demand curve, the Philippines committed to a 75 % greenhouse gas (GHG) emission reduction from 2020 to 2030 for the agriculture, waste, industry, transport, and energy sectors [29]. This implies that the industry sector should have an annual carbon footprint reduction of 7.5%. As a result, it was desired to reduce the carbon footprint of the extraction process by 7.5%. The composite curve was plotted such that the 7.5 % reduced carbon footprint of the process and corresponding total material and energy costs were the y- and x-values, respectively. The demand composite curve starts at the Cartesian origin and ends at the x- and y-values. After the material-based, energy-based, and demand composite curves were plotted, carbon footprint intensity analysis was conducted. The carbon intensity (slope) refers to the ratio of the material or energy component's carbon footprint and cost. The carbon intensity of the material-based and energy-based segments was investigated. The one with the greater carbon intensity was subjected to carbon footprint reduction.

Sensitivity analysis

The effect of petroleum nut cost on the carbon intensity of the extraction process was evaluated. The material-based and energy-based carbon intensity of the extraction process was determined and evaluated when the cost of fresh petroleum nut varied from 0.017 USD/kg to 16.94 USD/kg. 16.94 USD/kg was the cost in March 2025 from small-scale production, which was considered the maximum cost since the unit cost of petroleum nut was expected to decrease upon the commencement of large-scale production. Petroleum nut price was selected as the sole independent variable for the sensitivity analysis due to its high degree of uncertainty and impact on the operating cost structure. Solvent recovery rates were not included since, for this baseline study, solvent recovery was considered as a controlled parameter defined by distillation column efficiency and thermodynamic limits. On the other hand, the effect on carbon intensity was investigated rather than carbon footprint, because the carbon footprint of petroleum nut was calculated based on the quantity used rather than its cost. Hence, petroleum nut pricing has no effect on carbon footprint. The trends of material-based and energy-based carbon intensities were observed with respect to petroleum nut pricing. The optimal petroleum nut price was determined using the elbow method, selecting the point at which a sharp increase in carbon intensity was observed. Since the petroleum nut price was expected to decrease over time, carbon intensity was expected to increase. Therefore, the point at which a sharp increase in carbon intensity occurred was used as the reference.

RESULTS AND DISCUSSION

Process model

Figure 1 shows the generated batch process model for the solvent extraction of PNO via DWSIM. At the start of the process, both the solvent (isopropanol) and dried petroleum nuts are at a room temperature of 32 °C. It enters a heat exchanger (Heat Exchanger 1) to be heated to 50 °C. Then, it enters an extraction tank with agitation to simulate the extraction process. Afterwards, it enters a centrifuge (CS-1) to separate the miscella and de-oiled cake. The Flory-Huggins model was used to model PNO solvent extraction. To continue, the solid residues are filtered out after the extraction process to generate a solid-free miscella in the centrifuge (CS-1). The miscella (Extract) then goes to a distillation column (Distillation 1) for the solvent recovery system of the process. In this stage, isopropanol is recovered. Afterwards, the solvent-free stream (Mix -4) enters another distillation process (Distillation 2) for the water removal system. The latter stream contains water that needs to be removed according to the biodiesel standard of at most 0.05 % by mass moisture content. The distillation column was designed such that the moisture content of the PNO (Oil 1) is 0.05 %. The cooler (CL-1) was included in the process model to show that extracted PNO cools to room temperature in the storage tank. Note that the extracted oil is cooled naturally and without any cooling equipment. The oil recovery at the end of the process is 98.62 %. The value is comparable with the oil recovery of rubber seed oil at 95.12 % using a small-scale commercial screw press **[30]** and Brazil nut kernel oil at 90.58 % using a laboratory-scale pressurized isopropanol/ethanol solvent extraction **[31]**.

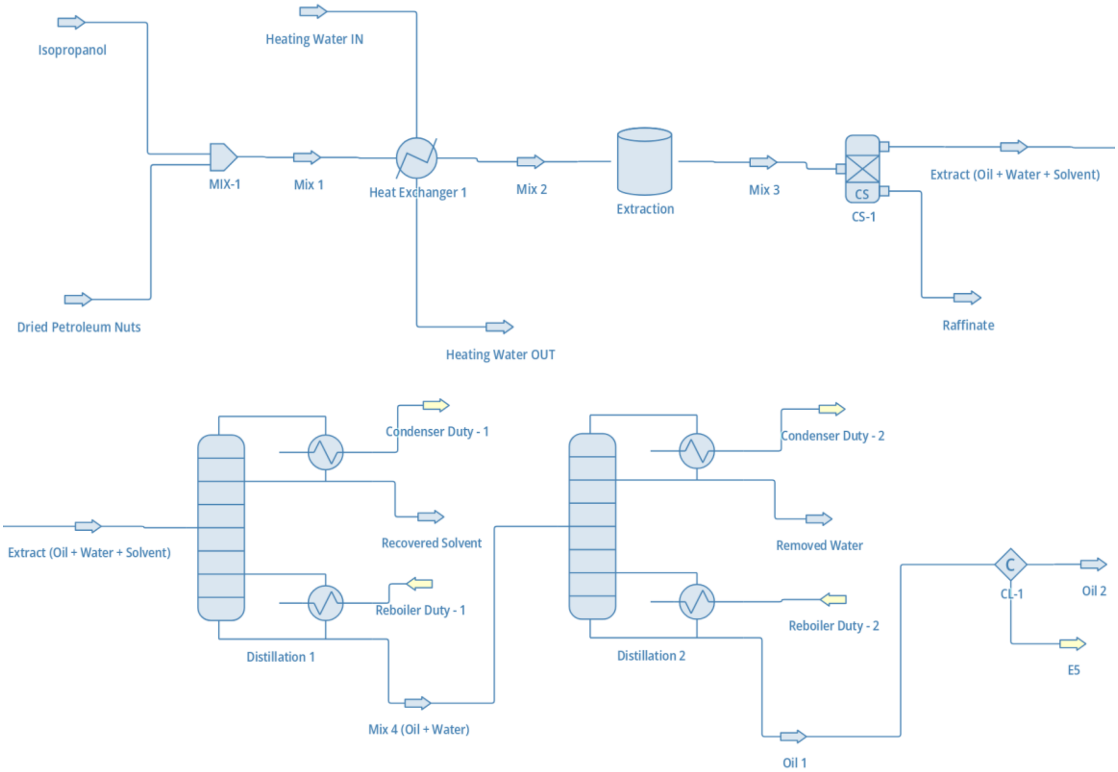

Figure 1. Process flow of the petroleum nut oil solvent extraction from DWSIM

The density of the extracted petroleum nut oil (from the process model) was 825.75 kg/m^3 at 20 °C. The density is comparable with the experimental density obtained by another study **[2]**, which is 916.2 kg/m^3 for PNO.

The Flory-Huggins model was used to calculate the retention factor of each compound, which was used to calculate the amount of solute in the solid and solvent phases after extraction. It incorporates the Hansen solubility parameters of the compounds to determine specific amounts that went to the solid and solvent phases. The model generated comparable oil recoveries to experimental runs in the extraction of rosmarinic acid from *Orthosiphon* **[18]**, which indicated good accuracy of the model. Table 6 shows the distribution of the compounds in the solid and solvent phases. It can be observed that the majority of the oil components (linoleic acid, myrcene, and alpha-pinene) were in the solvent phase.

Table 6. Distribution of compounds in the solid and solvent phases

Compounds	Amount in Solid Phase [kg/day]	Amount in Solvent Phase [kg/day]
Isopropanol	2,401.84	69,051.26
Linoleic Acid	28.27	3,270.60
Myrcene	25.07	2,935.95
Alpha-pinene	31.53	2,781.41
Water	805.15	13,909.07

It can be explained by the closeness of the oil components' Hansen solubility parameters with the solvent's total solubility parameter, because liquids with similar solubility parameters tend to be miscible [16]. Table 7 shows the calculated total solubility parameters of the compounds. These were calculated using Equation 3.

Table 7. Total solubility (Hansen solubility) parameters of compounds

Compound	δ_t [MPa$^{0.5}$]
Isopropanol	23.58
Linoleic Acid	19.89
Myrcene	16.23
Alpha-pinene	17.28
Water	47.81
Solid	25

The solubility parameter distance (Ra) between the solvent and oil components was small enough for the solvent to extract most of the oil components. Small Ra values suggest good miscibility between the solvent and solutes [18]. Table 8 shows the solubility parameter distance of solutes with respect to isopropanol, which were calculated using Equation 6. Therefore, the generated process model via DWSIM is considered a valid representation of PNO extraction.

Table 8. R_a values of solutes with respect to isopropanol

Compound	R_a [MPa$^{0.5}$]
Linoleic Acid	10.89
Myrcene	14.90
Alpha-pinene	14.15
Water	27.73

Material and Energy Consumptions and Costs

Table 9 shows the material and energy consumption and costs of the extraction process. The cooling water had the highest consumption among the components, followed by steam. The cooling water was used for the condensers in distillation operations. The material component was more expensive than the energy component, due to the high cost of the petroleum nut. Note that the cost considered here is still from small-scale production. The most expensive energy component was the generation of steam. It was also found that the total cost of extraction was 1,032,812.42 USD/day. The production capacity of the solvent extraction plant is 8,880.90 kg/day of PNO. Hence, the cost of PNO was estimated as 116.30 USD/kg.

Table 9. Material and energy consumption and cost

Component	Consumption [unit/day]	Cost [USD/day]	Cost (Material vs Energy) [USD/day]
Fresh petroleum nut [t]	55.00	948,835.29	1,012,162.16
Isopropanol [t]	71.45	63,326.87	
Steam [t]	1,252.46	17,437.11	20,650.26
Cooling Water [t]	2,866.83	2,618.36	
Electricity [kWh]	566.14	112.62	
Diesel [t]	0.45	482.17	
Total			1,032,812.42

Carbon Footprint Analysis

Tables 8 and 9 show the necessary inputs of the material-based and energy-based source composite curves following the methodology described in the previous section. Carbon intensity is defined as the ratio of carbon footprint and cost and can be obtained by getting the slope of the graph. Note that the material-based composite curve cost is followed by the energy-based composite curve. The energy-based composite curve was plotted from the terminal point of the material-based composite curve, and not from the origin. Figure 2 shows the source composite curve. It can be observed that the energy-based source composite curve has a steeper slope than the other. It can be inferred that the energy-based composite curve is more carbon-intensive (has a steeper slope) than the material-based curve. The dashed line in Figure 2 represents the carbon intensity of both components. Therefore, the energy component was prioritized for carbon footprint reduction analysis (Table 10).

Table 10. Material and energy carbon footprints

Component	Carbon Footprint [kg CO_2/day]	Carbon Footprint (Material vs Energy) [kg CO_2/day]
Fresh petroleum nut	8,619.55	125,088.09
Isopropanol	116,468.54	
Steam	15,087.89	18,006.75
Cooling Water	1,077.93	
Electricity	430.27	
Diesel	1,410.66	
Total		143,094.84

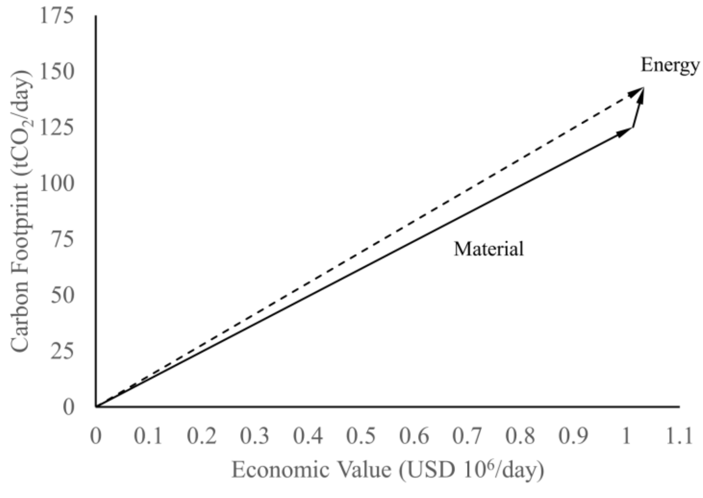

Figure 2. Source composite curves

On the other hand, the demand composite curve was generated from the desired 7.5 % carbon footprint reduction (10,732.11 kg CO_2/day) based on the total carbon footprint. Figure 3 shows the source and demand composite curves generated. It can be observed that the demand composite curve is below the source composite curve. The vertical gap between the two curves is equivalent to the desired 7.5 % carbon footprint reduction. The goal was to achieve the desired reduction by developing strategies to reduce the carbon footprint of the energy component, since it is more carbon-intensive than the material component.

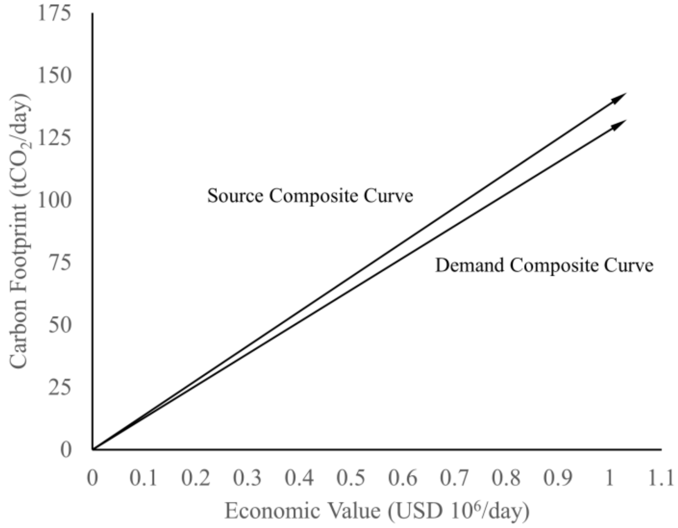

Figure 3. Source and demand composite curves

The energy-based composite curve was decomposed by plotting its internal and external segments separately, as shown in Figure 4. It can be observed from Figure 4 that the external energy component was more carbon-intensive (has a steeper slope) than the internal energy component. Hence, the external energy component requires more attention than the internal energy component. However, since the internal energy component has a higher overall carbon footprint, the proposed carbon footprint reduction strategy focused on the internal component, specifically steam generation. Therefore, the internal component was the hotspot for carbon footprint reduction.

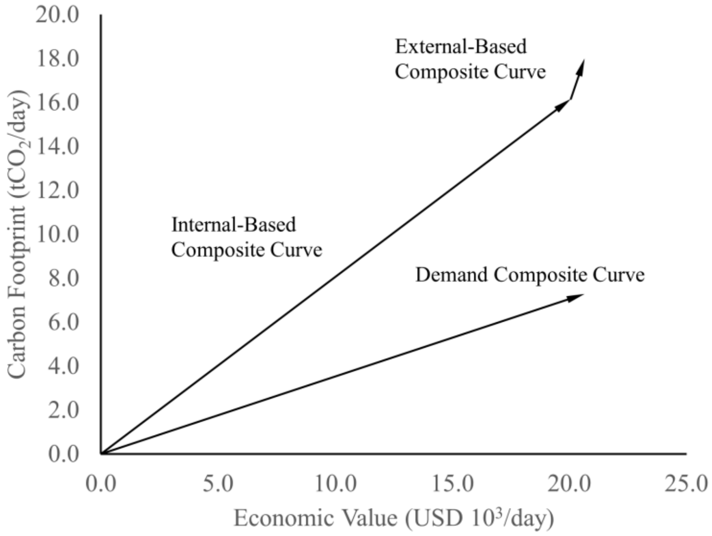

Figure 4. Internal- and external-based energy composite curves

The proposed carbon footprint reduction strategy was to use the de-oiled petroleum nut cake (DPNC) as solid fuel (as briquettes) for the boiler to generate steam. Steam production using DPNC briquettes as fuel was investigated to check if the proposed reduction measure can achieve the desired 7.5 % reduction. The results show that 29,320.22 kg/day of steam can be generated, with a carbon footprint of 5,118.72 kg CO_2/day, when DPNC briquettes were used as fuel. This strategy reduces the total carbon footprint of the energy component from 18,006.75 to 12,887.43 kg CO_2/day (28.43 % reduction).

Figure 5 shows the adjusted internal-based composite curve after the carbon footprint reduction strategy took effect. It is important to note that only the internal component was adjusted (steam generation), and the externally based composite curve was not adjusted. The adjusted internal-based composite curve now has a less steep slope than the original, as shown in Figure 5.

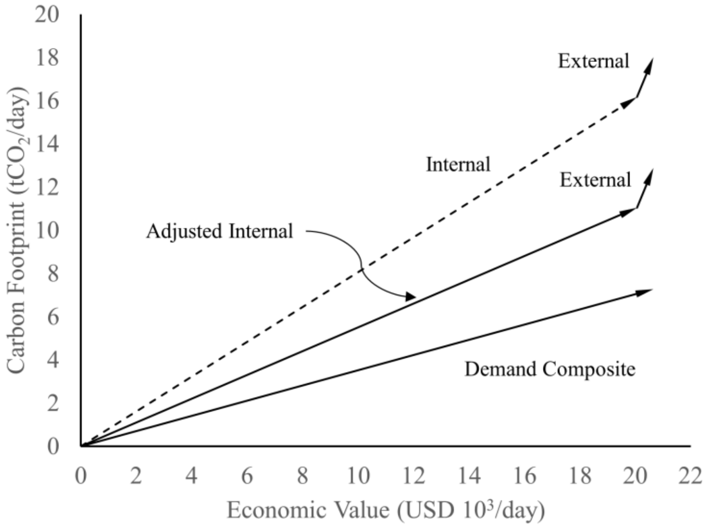

Figure 5. Adjusted internal-based energy composite curve

Figure 6 shows the adjusted source composite curve after carbon footprint reduction. It can be observed that because of the proposed carbon footprint reduction strategy, the energy-based source composite curve shifted down, which also caused the source composite curve to adjust accordingly. The total carbon footprint of the extraction process was reduced by 3.60 %. It did not achieve the desired 7.5 % reduction. However, it was about half of the desired reduction. A 3.60 % carbon reduction can be considered substantial when the scale of the operations is considered.

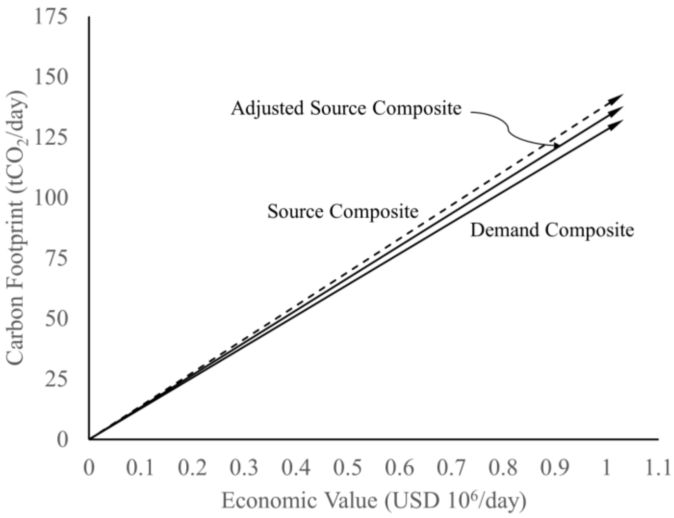

Figure 6. Adjusted source and demand composite curve

Sensitivity Analysis

Figure 7 shows the effect of petroleum nut pricing on material-based and energy-based carbon intensity. It can be observed that the energy-based carbon intensity was not affected by petroleum nut pricing. Carbon intensity is defined as the ratio of carbon footprint and cost. Since petroleum nut was not included in the energy component, neither its carbon footprint nor price influences the energy-based carbon intensity. On the other hand, since petroleum nut is a material component, the material-based carbon intensity was significantly affected by petroleum nut pricing. Results show that decreasing the petroleum nut cost increases the carbon intensity. This trend was anticipated, as there is an inverse relationship between cost and carbon intensity. In addition, results indicate a sharp increase in the carbon intensity of the material component when the unit cost of petroleum nut approaches approximately 2.54 USD/kg from 16.94 USD/kg.

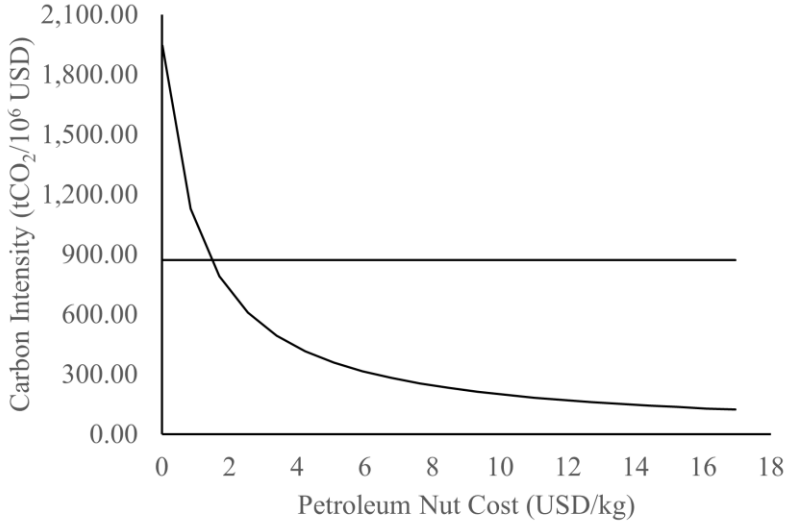

Figure 7. Effect of Petroleum Nut Pricing on Carbon Intensity

Using the elbow method, it can be concluded that a unit cost of 2.54 USD/kg of fresh petroleum nuts is the optimum price of petroleum nut with respect to material-based carbon intensity. It is important to note that this does not imply a reduction in carbon footprint. The carbon footprint of petroleum nut is still the same, since the carbon footprint of petroleum nut was calculated based on the quantity used rather than its cost. The change in petroleum cost was the only factor that caused the material-based carbon intensity to shift. As a result, the optimum price only implies a reduction in carbon intensity. The price of petroleum nut in March 2025 was 16.94 USD/kg. It can be reduced to the optimal cost of 2.54 USD/kg through efficient farming. Optimizing fertilizers, plant protection, buildings, farm equipment, and machinery, and labor can achieve a sustainable cost of crop cultivation [32].

CONCLUSION

A solvent extraction process model was designed using DWSIM based on the Flory-Huggins model to predict the separation of components. It applied the Hansen solubility parameters to predict the retention factors of the oil components. The small Ra values of oil components with respect to the solvent also suggested a high oil yield. Material and energy balances were performed using the process model in DWSIM. Calculations were conducted to determine the material and energy consumption. The total material and energy cost of a PNO solvent extraction plant with a production capacity of 8,880.90 kg/day is 1,032,812.42 USD/day. On the other hand, the total carbon footprint was found to be 143,094.84 kg CO_2/day. The carbon intensity method was used to identify hotspots for carbon footprint reduction. The carbon intensity of the material and energy components was investigated. The energy component was more carbon-intensive. Therefore, it was identified as a hotspot for carbon footprint reduction. A carbon footprint reduction of 7.5 % was targeted, corresponding to the Philippines' national objective of achieving a 75 % reduction in GHG emissions from 2020 to 2030. The proposed carbon footprint reduction strategy was to use the DPNC as fuel (as DPNC briquettes) to generate steam. Approximately 3.60 % carbon footprint reduction can be achieved with the proposed strategy. About half of the desired carbon footprint reduction (7.5 %) was achieved; hence, the proposed strategy was effective. The impact of petroleum nut pricing on carbon intensity was examined via sensitivity analysis, as it was identified as a significant factor influencing the carbon intensity of the material component. 2.54 USD/kg of petroleum nut is the optimal price of petroleum nut via the elbow method. A limitation of the proposed process assumes batch processing; therefore, a dynamic simulation of the extraction process would be a better representation of the process for future work. This study specifically applied the Carbon Footprint Intensity Method to account for carbon footprint relative to economic cost. While this method is similar to the graphical concepts of Pinch Analysis by using composite curves, it is distinct from thermodynamic heat integration. This study did not implement a Heat Exchanger Network synthesis, and the reported energy values reflect the heating and cooling requirements prior to heat recovery. Future work should explore other strategies to reduce the carbon footprint of the proposed extraction plant. Additionally, this study assumed a constant high-efficiency solvent recovery based on theoretical equilibrium. Future studies should investigate the sensitivity of the process to varying solvent recovery rates. This study adds to the growing literature of alternative renewable energy sources to produce biodiesel and high-value chemicals. The study demonstrates the effectiveness and simplicity of the carbon footprint intensity in determining hotspots for carbon footprint reduction in process industries.

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