

Article

Prioritizing CP Actions towards Circularity by Combining LCA and Energy in The PE Production Chain

G. Bustamante¹, B. F. Giannetti^{1,2}, F. Agostinho^{1,2}, G. Liu^{2,3} and C.M.V.B. Almeida^{1,2}

¹ Laboratório de Produção e Meio Ambiente, Programa de Pós-Graduação em Engenharia de Produção, Universidade Paulista, R. Dr. Bacelar 1212, São Paulo, Cep 04026-002, Brazil

² State Key Joint Laboratory of Environment Simulation and Pollution Control, School of Environment, Beijing Normal University, Beijing 100875, China.

³ Beijing Engineering Research Center for Watershed Environmental Restoration & Integrated Ecological Regulation, Beijing 100875, China.

Abstract: Petrochemicals, which convert oil and gas into products such as plastics, are fundamental to modern societies. Chemists recognize their role in the design of materials and the adverse effects that these may have on the environment, preventing sustainable development. Several methodological frameworks and sustainability assessment approaches have been developed to evaluate the resources used in the petrochemical sector in terms of environmental costs. A combination of Life Cycle Assessment and Energy Accounting - to assess the environmental support for resource use - is applied in this study of the PET production chain in Europe. The Unit Energy Values of several intermediates are calculated or updated to facilitate discernment of the quality of energy used and the processes' efficiency. Several routes for synthesizing renewable para-xylene and ethylene glycol from biomass are discussed and confronted with the efforts focused on recycling and recovering the final product providing concurrently a procedure and a valuable data set for future CP actions. The results show that understanding the efficiencies changing across the production chain may help stakeholders make wise choices as to where and when interventions to promote a circular economy are most effective along a petrochemical production chain.

Keywords: resource efficiency; productive chain trade-offs; decision making

1. Introduction

Modern industry requires different inputs to support production and profit. In particular, the chemistry sector faces numerous challenges as it contributes to almost all raw materials transformations into finished products. The sector's decisions directly affect the exploitation of natural resources and generate pollution with consequences to humanity at the societal/environmental dimensions [1]. In parallel, the current economy is still based on a linear model in which resources are extracted according to the production demand and consumption patterns. In addition, plastics production is more and more challenged to cater to an increasing population with non-renewable resources while controlling the adverse impacts on the environmental capacity of support. Such an economic system is indubitably not sustainable. It is already identified by global consensus as a major cause of local and global problems such as food/energy/water scarcity, climate change, and biodiversity loss [2,3]. It is urgent to let sustainability awareness and economy evolve together [4,5] to ensure that finite resource exploitation occurs under the best conditions allowed by the current technological/methodological development level.

Circular economy (CE) can play several crucial roles under this standpoint as a stimulating economic model that may help to preserve materials and products with high utility and value [4]. Geissdoerfer et al. [6] highlighted CE to be a required posture toward sustainability, as it may impose a regenerative structure that minimizes material and energy use, emissions, and wastes, by decelerating and closing the resource loops, the

two essential practices that make CE different from the linear economy [7]. In particular, slowing happens when long-life goods and product-life extension solutions are designed, and the use time of products is extended and/or intensified, contributing to slowing down the resource flows. When loops between end-of-life and production are closed, post-use products are recirculated within the life cycle, and low-burden resources are used to produce secondary raw materials [7]. Through those two practices, CE may satisfy the principle that the planet is a closed system with limited ability to support the increasing population growth and tolerate environmental degradation [8,9]. The economy and the environment need, therefore, to co-exist to preserve the earth's carrying capacity [8,9] by adopting, implementing, and spreading sustainability-oriented strategies [10] and to effectively help the transition to a carbon-neutral CE [10,11].

The petrochemical sector is responsible for diverse environmental impacts that depend upon the amount of non-renewable resources usage and the volume of pollutants released, damaging if directly discharged into the environment, even without an immediate impact [12]. Along the petrochemical production chains, nature and the human systems invest materials, energy, and services in each petrochemical product supplied for societal use. The plastics chain was recognized in the [10] as posing sustainability challenges that demand serious, all-inclusive, and organized CE-based actions. The EU Strategy for Plastics has developed a comprehensive set of initiatives to respond to the pressing global need to deal with plastics' end-of-life and to governments and companies pursuing sustainability goals using CE. Under this perspective, evaluating and improving the relevant environmental issues associated with plastics' life cycle may help meet such goals [10].

The most common polyester among plastics is polyethylene terephthalate (PET), with nearly 70 million tons supplied yearly for packaging and textiles [13]. Several contributions to altering the linear resource-depleting industry to a resource-valuing one have risen [14], especially regarding the use of recycled PET to replace petrochemical PET, contributing toward a circular PET economy. There are options such as waste-to-material through mechanical recycling [15,16], chemical recycling [17-19], and decomposition into fibers or smaller molecular components using sub- and supercritical fluids [20,21] or hydrolyzing enzymes [22]. There are also proposals to use flakes made of post-use bottle-derived PET as an insulating material for building thermal panels [23] and other construction materials [24]. Waste plastic developed into one of the most concerning environmental problems [25] and a central issue in waste management [26], considering the growth in production and fast consumption of the final products [27]. Thus, most efforts to insert the PET chain into the circular economy are focused on recycling and recovering the final product. However, these efforts to improve circularity are still marked by complexities and uncertainties [28], which should be managed and accounted for by practical and multidisciplinary tools that allow proper certification [29], creating standards and labels to ensure accurate decision-making. There is a need for assessing quantitatively if the solutions proposed to make the petrochemical sector chain circular effectively reduce the environmental burden or if they only alleviate the disposal-side and cause damages in other parts of the production chain or other parts of the environment. The investment to improve circularity, reducing the use of energy and materials, may be discriminated against and accounted for through the application of assessments methods capable of supplying quantitative indications to decision-makers.

Sustainability evaluation methods may help decision-makers ponder upon informed Cleaner Production (CP) choices on ecologically responsible procedures in production chains, mainly when their activities occur at the society/nature interface. The sustainability assessments supported by systematical and rigorous scientific frameworks and wide-ranging methods such as LCA (Life Cycle Assessment) and EmA (Emergency Accounting) are necessary to assist with environmental and economic sustainability.

LCA ponders on the relation of processes with the environment, which acts as sink and source and is based on inventories to develop indices connected to impact categories

such as global warming. This method has been widely used to estimate the environmental load inflicted by by-products and processes of the petrochemical industry [30,31], and the most complete and organized source of data on this sector is available on the PlasticsEurope website, a pan-European association that represents European manufacturers. The LCA-based eco-profiles [32, 33] provide information on market data, education, publications, but the authors also focused on the development of mathematical models to optimize petrochemical complexes by combining economic and environmental criteria [34,35], and the effects of replacing PET as packaging material [36,37].

EmA associates resource inflows to the Unit Energy Values (UEVs) that evidence the requirement for nature's support per resource unit. UEVs can be used to value and compare products on the same basis [38] and are useful indicators to estimate the environmental efficiency of production processes. Accounting for the work performed by the biosphere to produce a resource, the UEVs inform the extent to which the environmental support for natural resource generation converts into the final product. Lower UEVs suggest a higher resource use efficiency [39]. EmA also appeared as an option to assess the environmental performance of the petrochemical sector, accounting for the contributions from nature and from the man-made production chain evidencing the quantities of energy and materials, directly or indirectly, required to obtain products and services [38]. Oil-based production routines were evaluated by Bastianoni et al. [40], who calculated the unit energy values (UEVs) of natural gas and crude oil, and subsequently, the UEVs of the liquid petroleum products [41], which were used to estimate the energy contribution of naphtha for different ethylene production processes [42]. Brown et al. [43] divided crude oil and natural gas production into two formation phases: organic matter generated by tidal, solar, and geothermal energies and petroleum generated by geothermal energy. The calculated UEVs give an idea of the environmental load imposed by the exploitation of these resources on the donor-side, that is, the available energy required to supply these resources to the chemical industry and, ultimately, to societal use.

Previous efforts to integrate EmA and LCA combined the extensive LCA inventories and rules with the more far-reaching conceptual framework of the EmA approach to make environmentally sensible decisions in engineering processes would benefit from combining the two methods [44]. However, the effort to integrate structure and software showed some barriers challenging to overcome, such as conflicting specific goals, allocation rules, spatial and time scales [45-48], although authors agreed that EmA could benefit by expanding the accessible LCA databases [49] and permitting a broader understanding of the existing systems and their potential improvements scenarios [50].

Under the circular viewpoint, the combination of life cycle thinking and energy/exergy evaluations was considered suitable to subsidize the chemical sector for developing innovative value-added chemical products produced from waste-derived materials [51]. In this context, Almeida et al. [52] applied the energy synthesis combined with LCI data on the aluminum and PET packaging life cycles, including the recycling options contributing to the processes and materials selection during the product design stage or to establish public policies for recycling options [53]. UEV values close to those calculated by Bastianoni et al. [41] and Brown et al. [43] were obtained by an LCI-based unit energy values of naphtha calculated by Bustamante et al. [54].

The literature review suggests that combining EmA and LCA may improve the evaluations of the environmental performance and the choice of CP actions by (1) integrating opposed perspectives: the donor/supplier-side with a user/receiver-side and (2) including EmA's concept of the environmental work necessary to obtain a product escalating the spatial and time scales of LCA [44].

In this work, a course of action combining EmA and LCA provides an additional step toward assessing and documenting procedures for CE, considering some of the

complexities and uncertainties involved in sustainability assessments. Results will thus contribute by (1) underscoring the use of LCA inventories to contribute to CE; (2) providing new values of the UEVs of PET and intermediate chemicals and facilitating discernment of the quality of energy used and the processes' efficiency; (3) providing an alternate method for calculating UEVs using LCA and EmA combination through the investigation of the PET resin production chain; (4) helping to prioritize actions towards closing loops to achieve a cleaner/circular petrochemical industry.

2. Methods

LCA is a well-recognized assessment method for registering and assessing inputs, outputs, and the prospective impacts over its entire life cycle [55,56]. The LCA structure includes the definition of scope, inventory, impact assessment, and interpretation. For the interpretation phase, the method offers indicators associated with categories of environmental impacts, such as climate change, acidification, and land use.

Raw data of the PET production chain were collected using the LCI databases from Plastics Europe [33,57], which include all flows that contribute to the processes from the extraction of natural resources to obtaining 1 kg of product "at gate" set to be used in the next stage (representing the average of European industrial production) or to obtain 1kg finished product ready for delivery to consumers/users. Therefore, the LCI database and the Eco-profiles follow the instructions of the ISO 14040-44 standards series [33,57].

Following the growing attention on the embodied energy accounting system and the interface energy/environment [58-60], EmA was introduced by H.T. Odum to express the work done by nature to obtain every biosphere element, with the idea of expressing all resource flows in the same unit (solar energy joules, *sej*). Emergy is the available energy directly or indirectly required to generate a product or service [38]. The total emergy is calculated by the sum of each input's energy content multiplied by its UEV (*sej/unit*), which denotes the emergy invested to generate one flow unit. UEVs refer to a geobiosphere energy baseline (12.0 E+24 *seJ/yr*) that results from the sum of the annual emergies - solar, gravitational, and geothermal - that drive the biosphere [61] and were calculated by dividing the total emergy required to produce a given output by 1 unit of this output.

2.1. Calculating UEVs from LCIs of the explored petrochemicals

Regarding the target products, it was considered that PET is most commonly produced by the polycondensation reaction between purified terephthalic acid obtained from para-xylene - made from monomers of benzene, toluene, and xylene isomers (BTX), and ethylene glycol [62] - produced from ethylene by the steam cracking of hydrocarbons through the ethylene oxide intermediate [63].

The investigated chemicals were tracked back using the PlasticsEurope [33,57] inventories to recover the original inputs of the PET production chain. These Eco-profiles follow the instructions for calculating the information following the ISO 14040-44 standards [33,57].

The premise for the UEVs calculation for each output was established considering no allocation [64] - accounting for all flows of natural resources contributing to obtain 1 kg of product "at gate," that is, inventories were directly used to convert LCIs raw data into energy values. In this way, the energy calculations agree with the standards of the LCA procedure. (Eqs. 1 and 2).

$$U = \sum E_i \times UEV_i \quad (1)$$

where U is the total energy (*sej*), E_i is the available energy of the i -th input flow - material and energy delivered to the system. UEV_i is the energy required to obtain one unit of that input flow (Eq. 2). The quantity of every input is multiplied by its corresponding UEV resulting in the energy needed to produce 1 kg of output.

$$UEV_j = U/Y_j$$

(2)

where: UEV_j is the UEV of the product j , U is the total energy, and Y_j is the yield of the process, that is, the products energy or mass content.

The production flow involving the nine investigated chemicals (crude oil, naphta, xylene, ethylene, p-xylene, ethylene oxide, ethylene glycol, purified terephthalic acid and PET) are shown in Fig. 1 in a conventional flow-chart. The complete tables for all materials are available in Supplementary Materials, tables S1-S8.

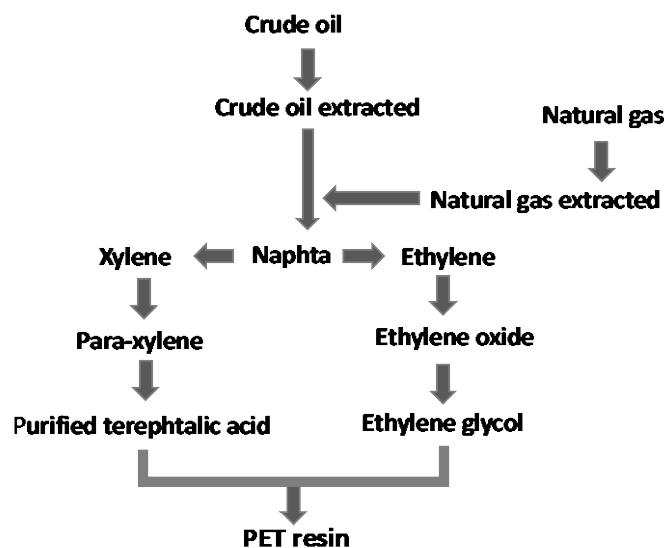


Fig. 1. The production flow of PET resin involving the nine investigated intermediate inputs (crude oil, naphta, xylene, ethylene, p-xylene, ethylene oxide, ethylene glycol and purified terephthalic acid).

For each chemical product, the LCIs include contributions from different material flows, energy, fuels, and metals, among others, and the resulting energy tables provide an estimate of the energy directly or indirectly used to obtain these flows. The flows relative to the facilities' construction stage and maintenance were not accounted for since their influence on energy results is low [41,42]. Similarly, entries for labor and services were not included, because these flows are country-specific and depend upon local economic and social structures. When labor and services are included, results also become country-specific, and the overall scope of evaluating the technical processes becomes compromised [65].

3. Results

Results are presented in two steps: (3.1) the calculation of LCI-based UEVs and (3.2) the potential use of UEVs to support decision-making toward a circular economy.

3.1. Calculations and analysis of the LCI-based UEVs

LCI-based UEVs of PET production and of nine selected intermediates (crude oil, naphta, xylene, ethylene, p-xylene, ethylene oxide, ethylene glycol, and purified terephthalic acid - with detailed calculations in the Supplementary Material, Tables S1-S8) are shown and compared with UEVs retrieved from previously published papers.

The LCI-based energy for PET is shown in Table 1. Local renewable resource flows provide less than 1% to the total energy of PET production. The resulting UEV of PET is 5.94E+09 sej/g, with crude oil contributing the most (71.4%), followed by natural gas (19.2%).

Table 1. LCI-based* energy required to produce 1 kg of PET resin.

INPUTS	Unit	Quantity*	UEV**	unit	Energy
1 Energy, gross calorific value, in biomass	MJ	4.22E-01	6.75E+04	seJ/J	2.85E+10
2 Peat, in ground	kg	9.39E-07	3.19E+04	seJ/J	2.92E+05
3 Wood, primary forest, standing	m3	1.04E-06	1.04E+04	seJ/J	1.22E+08
5 Energy, gross calorific value, renewable	MJ	4.55E-01	1.02E+05	seJ/J	4.63E+10
6 Energy, hydro	MJ	3.39E-01	1.35E+05	seJ/J	4.56E+10
7 Energy, gross calorific value, in lignite	MJ	1.39E+00	6.22E+04	seJ/J	8.63E+10
8 Aluminium, 24% in bauxite, 11% in crude ore, in ground	kg	1.14E-05	5.40E+09	seJ/g	6.15E+07
9 Barite, 15% in crude ore, in ground	kg	2.67E-05	1.68E+09	seJ/g	4.49E+07
10 Basalt, in ground	kg	3.61E-10	7.56E+09	seJ/g	2.73E+03
11 Borax, in ground	kg	1.63E-10	1.68E+09	seJ/g	2.75E+02
12 Cadmium, 0.30% in sulfide, Cd 0.18%, Pb, Zn, Ag, In, in ground	kg	6.54E-12	3.40E+13	seJ/g	2.22E+05
13 Calcite, in ground	kg	9.02E-03	1.68E+09	seJ/g	1.51E+10
14 Carbon, in organic matter, in soil	kg	3.34E-08	2.77E+09	seJ/g	9.25E+04
15 Chromium, 25.5% in chromite, 11.6% in crude ore, in ground	kg	1.13E-05	1.50E+11	seJ/g	1.70E+09
16 Chrysotile, in ground	kg	2.97E-07	1.68E+09	seJ/g	4.98E+05
17 Clay, unspecified, in ground	kg	1.95E-04	4.80E+09	seJ/g	9.39E+08
18 Coal	MJ	2.45E+00	5.71E+04	seJ/J	1.40E+11
19 Cobalt, in ground	kg	1.80E-04	1.30E+11	seJ/g	2.34E+10
20 Colemanite, in ground	kg	4.53E-09	1.68E+09	seJ/g	7.62E+03
21 Copper, in ground	kg	1.07E-06	9.80E+10	seJ/g	1.05E+08
22 Diatomite, in ground	kg	2.00E-13	1.68E+09	seJ/g	3.36E-01
23 Dolomite, in ground	kg	2.53E-06	1.85E+10	seJ/g	4.69E+07
24 Feldspar, in ground	kg	2.07E-12	1.68E+09	seJ/g	3.48E+00
25 Fluorine, in ground	kg	8.13E-06	1.68E+09	seJ/g	1.37E+07
26 Fluorspar, 92%, in ground	kg	8.37E-06	8.38E+08	seJ/g	7.02E+06
27 Gas, natural, in ground	MJ	1.67E+01	6.83E+04	seJ/J	1.14E+12
28 Gold, in ground	kg	2.44E-17	5.00E+11	seJ/g	1.22E-02
29 Granite, in ground	kg	2.07E-12	8.40E+08	seJ/g	1.74E+00
30 Gravel, in ground	kg	6.65E-03	8.40E+08	seJ/g	5.59E+09
31 Gypsum, in ground	kg	3.19E-09	2.85E+09	seJ/g	9.10E+03
32 Indium, 0.005% in sulfide, In 0.003%, Pb, Zn, Ag, Cd, in ground	kg	1.03E-13	4.03E+11	seJ/g	4.15E+01
33 Iron, 46% in ore, 25% in crude ore, in ground	kg	4.18E-05	1.20E+10	seJ/g	5.02E+08
34 Kaolinite, 24% in crude ore, in ground	kg	6.87E-07	1.68E+09	seJ/g	1.15E+06
35 Kieserite, 25% in crude ore, in ground	kg	1.69E-09	1.68E+09	seJ/g	2.84E+03
36 Lead, 5.0% in sulfide, Pb 3.0%, Zn, Ag, Cd, In, in ground	kg	4.31E-11	4.80E+11	seJ/g	2.07E+04
37 Magnesite, 60% in crude ore, in ground	kg	6.86E-07	1.68E+09	seJ/g	1.15E+06
38 Manganese, 35.7% in sedimentary deposit, 14.2% in crude ore, in ground	kg	3.15E-04	3.50E+11	seJ/g	1.10E+11
39 Mercury, in ground	kg	2.71E-08	4.20E+13	seJ/g	1.14E+09
40 Metamorphous rock, graphite containing, in ground	kg	8.31E-09	1.68E+09	seJ/g	1.39E+04
41 Molybdenum, 0.025% in sulfide, Mo 8.2E-3% and Cu 0.39% in crude ore, in ground	kg	4.75E-07	7.00E+11	seJ/g	3.32E+08

42	Nickel, 1.13% in sulfide, Ni 0.76% and Cu 0.76% in crude ore, in ground	kg	2.63E-05	2.00E+11	seJ/g	5.26E+09
43	Oil, crude, in ground	MJ	4.49E+01	9.45E+04	seJ/J	4.24E+12
44	Olivine, in ground	kg	7.05E-10	1.68E+09	seJ/g	1.19E+03
45	Pd,in ground	kg	1.13E-08	1.20E+11	seJ/g	1.36E+06
46	Phosphorus, 18% in apatite, 12% in crude ore, in ground	kg	3.25E-05	2.07E+10	seJ/g	6.71E+08
47	Potassium chloride, in ground	kg	4.02E-08	4.97E+09	seJ/g	2.00E+05
48	Pt, in ground	kg	1.95E-12	3.70E+11	seJ/g	7.20E+02
49	Rh, in ground	kg	1.74E-12	1.20E+12	seJ/g	2.09E+03
50	Rhenium, in crude ore, in ground	kg	4.83E-13	8.93E+12	seJ/g	4.31E+03
51	Rutile, in ground	kg	2.07E-12	1.68E+09	seJ/g	3.48E+00
52	Sand, unspecified, in ground	kg	5.61E-08	1.68E+09	seJ/g	9.43E+04
53	Shale, in ground	kg	6.13E-09	1.68E+09	seJ/g	1.03E+04
54	Silver, in ground	kg	6.51E-17	4.50E+11	seJ/g	2.93E-02
55	Sodium bromide, in ground	kg	4.40E-04	1.68E+09	seJ/g	7.39E+08
56	Sodium chloride, in ground	kg	1.30E-02	1.68E+09	seJ/g	2.19E+10
57	Sodium nitrate, in ground	kg	3.33E-15	1.68E+09	seJ/g	5.60E-03
58	Sodium sulphate, various forms, in ground	kg	2.24E-06	1.40E+09	seJ/g	3.13E+06
59	Stibnite, in ground	kg	2.71E-04	1.68E+09	seJ/g	4.55E+08
60	Sulfur, in ground	kg	4.60E-05	2.08E+10	seJ/g	9.58E+08
61	Talc, in ground	kg	9.79E-08	2.80E+10	seJ/g	2.74E+06
62	Tantalum, 81.9% in tantalite, 1.6E-4% in crude ore, in ground	kg	2.36E-17	1.70E+11	seJ/g	4.02E-03
63	Tellurium, 0.5ppm in sulfide, Te 0.2ppm, Cu and Ag, in crude ore, in ground	kg	3.20E-18	5.04E+13	seJ/g	1.61E-01
64	Tin, 79% in cassiterite, 0.1% in crude ore, in ground	kg	3.01E-11	1.70E+12	seJ/g	5.11E+04
65	TiO2, 54% in ilmenite, 2.6% in crude ore, in ground	kg	4.89E-06	3.82E+10	seJ/g	1.87E+08
66	Ulexite, in ground	kg	1.21E-17	1.68E+09	seJ/g	2.02E-05
67	Uranium, in ground	kg	6.78E-06	1.60E+11	seJ/g	1.08E+09
68	Zinc, 9.0% in sulfide, Zn 5.3%, Pb, Ag, Cd, In, in ground	kg	8.11E-07	7.20E+10	seJ/g	5.84E+07
69	Zirconium, 50% in zircon, 0.39% in crude ore, in ground	kg	3.25E-17	3.18E+10	seJ/g	1.03E-03
70	Magnesium, 0.13% in water	kg	3.73E-18	1.68E+09	seJ/g	6.26E-06
71	Water, cooling, unspecified natural origin	m3	5.12E-02	2.70E+05	seJ/g	1.39E+10
72	Water, lake	m3	1.52E-03	4.52E+05	seJ/g	6.85E+08
73	Water, process, unspecified natural origin	m3	4.20E-03	6.74E+04	seJ/J	1.18E+09
74	Water, river	m3	1.77E-03	3.41E+05	seJ/g	6.03E+08
75	Water, salt, ocean	m3	5.38E-05	5.36E+04	seJ/J	1.21E+07
76	Water, salt, sole	m3	1.24E-05	5.36E+04	seJ/J	2.79E+06
77	Water, unspecified natural origin	m3	2.97E-05	3.06E+04	seJ/J	3.80E+06
78	Water, well, in ground	m3	6.34E-04	6.89E+04	seJ/J	1.83E+08
					Energy	seJ
					UEV	seJ/g
						5.94E+12
						5.94E+09

*Inputs quantities as reported in the Ecoprofiles provided by PlasticsEurope [33,57]. Nomenclature of the inputs was kept as shown in the original Ecoprofiles to facilitate analysis and comparisons

**UEVs used for calculating the emergy of inflows were obtained from the literature and related to the baseline 12.0E + 24 sej/yr [61, 66].

Table 2 summarizes the results classifying the emergy inputs according to their contribution to the total emergy. Inputs were divided into crude oil, natural gas, energy, materials (mostly minerals and metals), and water. In regard to resource use, crude oil is clearly the main contribution to all products and, consequently, the main concern within the whole PET production chain. The contributions of natural gas go from 6% to xylene production to about 20% to PET resin. The energy supplied by different sources (including renewables, biomass, and hydroelectricity) contributes less than 6% to all products and the contributions of water and materials are lower than 2% in all cases. Details of the relative contributions of emergy inputs are available in Table S9 in Supplementary materials.

Table 2. Summary of the LCI-based* emergy required to produce PET resin and nine selected intermediates (crude oil, naphtha, xylene, ethylene, p-xylene, ethylene oxide, ethylene glycol, and purified terephthalic acid).

Emergy /(sej/kg)						
Table*	Product	Crude oil	Natural gas	Energy	Materials	Water
S1	crude oil	4,28E+12		1,93E+11	7,80E+07	2,19E+06
S2	naphtha	4,54E+12		2,08E+11	1,82E+08	8,30E+06
S3	xylene	4,87E+12	3,43E+11	9,15E+09	1,53E+10	3,24E+09
S4	ethylene	5,48E+12	8,46E+11	3,23E+10	3,82E+10	4,46E+09
S5	p-xylene	5,68E+12	4,17E+11	1,81E+10	2,48E+10	5,93E+09
S6	ethylene oxide	4,40E+12	7,54E+11	1,21E+11	1,10E+11	1,01E+10
S7	ethylene glycol	3,16E+12	5,74E+11	1,28E+11	1,15E+11	1,15E+10
S8	purified terephthalic acid	3,86E+12	7,56E+11	6,36E+10	3,08E+11	1,82E+10
1	PET	4,24E+12	1,14E+12	3,47E+11	1,95E+11	1,65E+10

*The complete tables are available in the Supplementary Material, S1-S8

Table 3 shows all the UEVs calculated in this study (see Supplementary Material) compared with UEVs from the published literature.

Table 3. Unit emergy values (in solar emergy joules per gram of product, sej/g) of intermediaries of the PET production chain calculated and compared with literature. All values are relative to the baseline 12.0E + 24 sej/yr [61,66], and mass/energy conversions used were: $4.19 \times 10^4 \text{ J/g}$ for oil, and $5.13 \times 10^4 \text{ J/g}$ for natural gas [41,42].

Product	UEV/ (E+09 sej/g)	UEV/ (E+09 sej/g)	Reference
	This work	Literature	
Crude oil	4.47	2.96	Bastianoni et al., 2009
Crude oil extracted		6.20	Brown et al., 2011
Natural gas		2.80	Bastianoni et al., 2009
Natural gas extracted		6.66	Brown et al., 2011
Naphtha	4.52	5.02	Sha et al., 2015
xylene	5.24		
ethylene	6.40	12.0	Sha et al., 2015
p-xylene	6.15		
ethylene oxide	5.40		

ethylene glycol	3.99		
purified terephthalic acid	5.00		
PET resin	5.94	26.1	Almeida et al., 2010

The LCI-based UEV of naphtha, for example is close to the value estimated by Sha et al. [42] who used the value reported by Bastianoni et al. [41] for petroleum liquid fuels multiplied by the calorific value of naphtha. Similar results were obtained in comparing the LCI-based UEVs with those estimated by [41,43] for crude oil. All UEVs vary within the same order of magnitude (E+09) and using the LCA database for all products may provide a more uniform inventory, which may partially minimize the problem of finding different values in the literature. The geographic location may influence due to the different kinds of electricity matrixes found in different countries. The variations in the calculated values may also vary according to technological levels between the systems considered by the LCIs published by other authors. For example, the PET resin production process in Brazil was found an intensive consumer of biosphere resources with a much higher UEV value when compared with the European production [52] (Almeida et al., 2010).

3.2. The potential use of UEVs to support CP actions towards circular economy

Higher UEVs values mean higher investment in environmental resources for the same amount of output, but UEVs may also be understood as measures of energy quality by expressing ratios between the quantities of the energy required per joule of the product [38] (Odum, 1996). From this point of view, transformity provides a scale of energy transformations that establishes a hierarchy - the higher the transformity of a product, the more resources it requires and the more valuable is this product. The calculated UEVs for the PET production chain indicate that the efforts to introduce the chain into the circular economy focused on recycling post-use PET bottles is positive, as they intend to keep the materials of highest quality (highest UEVs) circulating as long as possible. Figure 4 shows an estimate considering the mechanical recycling beverage packages in which recycled PET reaches 55% of total PET, as foreseen by Plastics-recyclers-europe [32] for 2030. Clearly, the energy required for packing with recycled materials is significantly reduced when compared to that which uses virgin materials at all stages of the production chain.

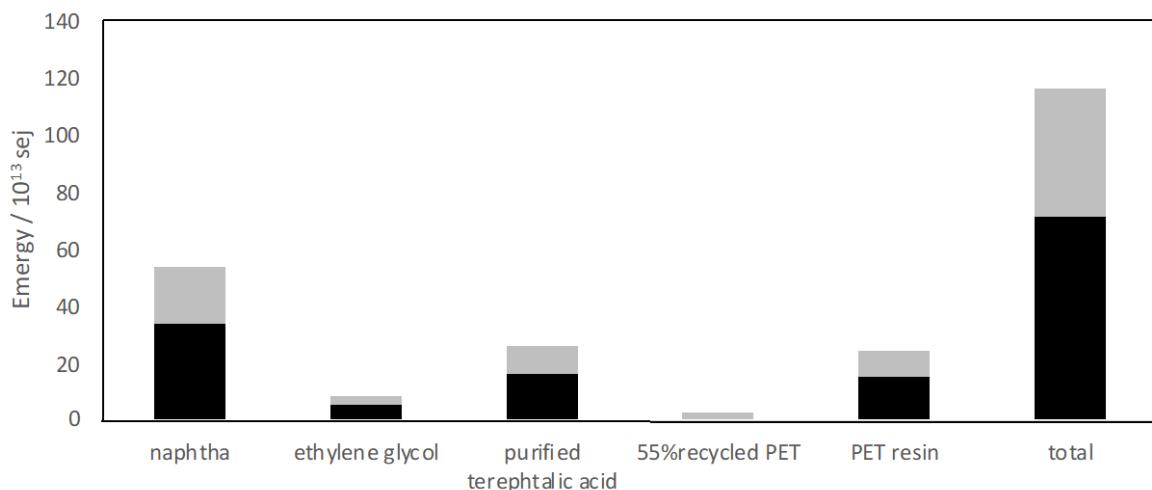


Figure 4. The potential effect of using 55% of recycled PET on the energy required to produce PET resin relative to 1000 L of beverage or 2 L PET bottles for the case of beverage packages mechanical recycling (for further details see [52,53]).

Despite the environmental load decrease in the overall life cycle, relative to the energy use and the naphtha savings, it is crucial to prioritize/identify opportunities for

improvements and changes considering the fast consumption of the final products in the case of PET packages [27], and the huge amounts of materials processed through the life cycle that continues to increase dissipative emissions. Shifting to a real circular economy for PET may help to close the loop preventing their way into landfills and protecting the marine environment against the (micro)plastic pollution [67].

4. Discussion

The obtained results highlight the importance of reliable databases for full and multidimensional sustainability assessment as well as for more studies about the resource use to produce chemicals in the petrochemical production network. The discussion is divided into two main subjects: (4.1) The importance of accurate and easy-to-calculate UEVs and (4.2) how this indicator may help to improve the circularity in the PET production chain.

4.1. *The importance of accurate and easy to calculate UEVs*

UEV is a measure of environmental efficiency. Higher UEV values mean lower environmental efficiency, which cannot be overlooked or ignored. This study sets up a foreseeable range for transformities of the petrochemical industry reducing the uncertainties in the selection of UEVs for energy analysis of the petrochemical industry and providing an alternative for future studies to expedite work on data collection. With the comprehensive data supplied by the PlasticsEurope database [33,57], UEVs were calculated for PET resin and nine selected intermediates (crude oil, naphtha, xylene, ethylene, p-xylene, ethylene oxide, ethylene glycol, and purified terephthalic acid). These chemicals are also used in other industrial processes. Ethylene glycol, for example, is an industrial compound used as antifreeze, fluid for hydraulic brakes, solvents, paints, other plastics, and cosmetics.

Therefore, an easy UEV calculation routine based on elementary flows from the LCIs may provide consistent UEVs for the evaluation of several other processes and avoid allocation since every calculated UEV derives from the elementary flows that contribute to the product or intermediate from the extraction of natural resources to obtaining 1 kg of product "at gate" ready to be used in the next process.

The combination of LCA inventories and EmA helps quantify and qualify changes in resource use and facilitate policy adjustment, the adoption of a CP practice over another, and monitoring changes.

4.2. *How UEVs may help to improve the circularity in the PET production chain*

The current most common supply chain is used to benchmark the system and evaluate CP options toward CE.

Instinctively, the reuse option or the adoption of returnable bottles is generally accepted by the scientific community as better than recycling [68, 69] since the more finished products circulate within their own production chain, the closer this chain will be to the natural ecosystem, and the lower will be the load inflicted to the environment [70]. However, some authors advise against reusing PET bottles due to the potential release of phthalate esters with endocrine-disrupting effects [71].

Exploring a different angle, several routes for the synthesis of renewable para-xylene from biomass have been explored with different accomplishment levels proposing a renewable PET by obtaining both para-xylene and ethylene glycol from biomass [72, 73], such as the Coca-Cola plant bottle, where ethylene glycol was partially obtained from sugarcane-derived bioethanol [74] or the paper bottle trial [75]. Both initiatives may potentially reduce the crude oil extraction by moving the PET production to another production chain based on agriculture, as shown in Fig. 3. These two options should be, however, deeply evaluated about their environmental performance and without forgetting the debate on the use of soil with its priority for food production [76]. In a good

start, Shah et al. [42] analyzed four ethylene production systems - from naphtha, natural gas or pine residue, and switchgrass bioethanol - using energy synthesis. The naphtha's UEV was found to be 2–3 times lower than the UEV of the biomass-based ethylene, and naphtha steam cracking was distinguished by high yields and high loads on the environment, while processes based on biomass showed low energy yield rates and lower environmental loadings. The trade-off lies between short-term profit and lower environmental loading ratios, but this kind of solution, severely accessed, may help to decouple PET production from fossil fuel depletion.

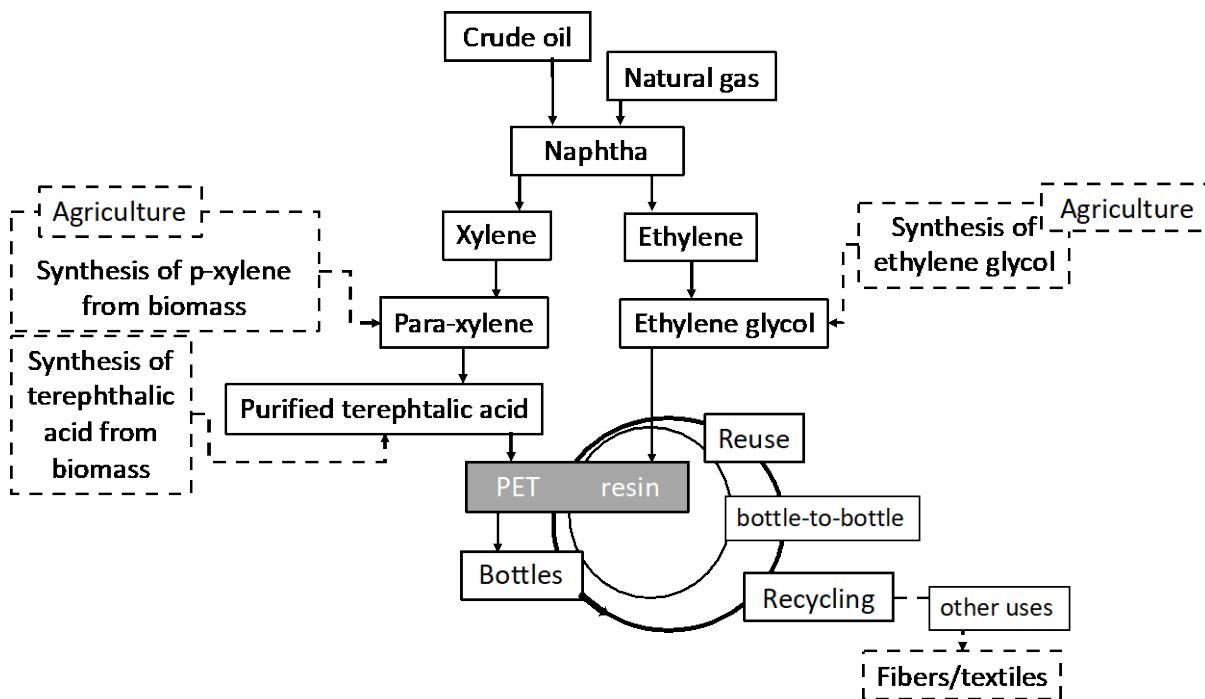


Figure 3. Potential routes to produce PET resin and some recycling options.

A third option lies in the chemical recycling [17,18] and PET decomposition into fibers or smaller molecules [20,21] to be used in different products such as the textile [77] or the construction industries [78]. These options extend the useful lives of these materials, but also open new fields for research on the disposal of the new products, and despite recycling itself is a good option to promote a circular economy in the sector, much research and work still need to be done for its effective implementation through waste management strategies [79,80].

In this context, the UEVs results that show a clear gap between the transformity values of basic materials and those of their derivatives indicate that not only actions targeting these derivatives may be more effective to move from the linear 'extract–make–dispose' model to the circular one, but also selecting the best route comparing the environmental support demand and seizing the energy savings due to the substitution of inputs, the combination of different supply chains, the reuse or recycle of waste or the effectiveness of management options. Figure 5 shows the different action fronts for the implementation of a and well-planned CE that may expand the results from the PET resin production chain to other production systems.

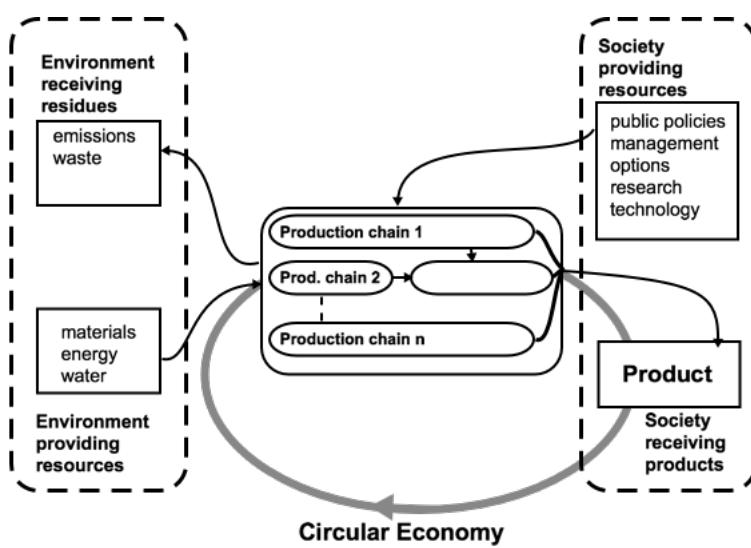


Figure 5. Required coordinate actions/assessments for the implementation of CE. Adapted from the SEctor SUstainability (5SEnSU) model [81].

The understanding of the efficiencies (UEVs) changing intra and inter several alternative production chains may help to assess the effect of cleaner production activities along each chain, of the circulation of the materials at the inter-firm or inter-chain levels and the potential to increase the resilience of the overall system. This kind of assessment, taking into account all sectors depicted in Fig. 5, may also give support to expanding existing synergies such as the reuse practices, the reduction of energy consumption, and the carbon footprint to transform the production chain from linear to closed loop. In addition, monitoring these efficiencies may also help to guide research and the search for new technologies, to establish and adjust public policies, management alternatives, and promote awareness among consumers.

5. Conclusions

Although the benefits of an enforced circularity of the petrochemical sector are well-defined, multidimensional sustainability issues and the variety of options for the transition towards increased recycling and innovative materials call for indicators capable to assess each proposal and prioritize actions toward closing loops discerning the quality of energy used and the processes' efficiency.

The PET production chain was explored from the standpoint of resources and energy use covering a selection of intermediate products. New UEVs for petrochemical commodities were estimated using LCIs databases (xylene, para-xylene, ethylene oxide, ethylene glycol, and purified terephthalic acid) establishing priorities and providing an indicator to interfere in the PET production chain.

Moving to a real circular economy is complex and cannot rely on single life cycles of chemical products but the chemistry sector as a whole, combining different production chains to replace the current linear approaches. For this, operational barriers to co-work among different sectors, such as the bio-based plastics sector with the petrochemical one, both supported by public policies and consumer awareness, to encourage the transition to a circular, sustainable, and well-designed production network. There is a need for this to be focused on given the short useful life of most plastics – packages in special – and their latent damaging impacts on the environment. The shift towards a circular economy for the plastics sector in which wastes are either reused, remanufactured, or recycled into old/new uses compels coordinated action. One of them is the understanding of the efficiencies (UEVs) changing across all life stages and all life cycles in a way that

shareholders can make well-versed judgments and choices as to where and when CP interventions are most effective.

Acknowledgments: The authors acknowledge the support of "Vice-Reitoria de Pós-Graduação e Pesquisa da Universidade Paulista (UNIP).

References

- [1] Gbededo, M.A., Liyanage, K., Garza-Reyes, J.A., 2018. Towards a Life Cycle Sustainability Analysis: A systematic review of approaches to sustainable manufacturing. *Journal of Cleaner Production* 184, 1002-1015.
- [2] Korhonen, J., Honkasalo, A., Seppälä, J., 2018. Circular economy: the concept and its limitations. *Ecological Economics* 143, 37-46.
- [3] Keijer, T., Bakker, V., Slootweg, J.C., 2019. Circular chemistry to enable a circular economy. *Nature Chemistry* 11(3), 190-195.
- [4] Ingrao, C., Faccilongo, N., Di Gioia, L., Messineo, A., 2018. Food waste recovery into energy in a circular economy perspective: A comprehensive review of aspects related to plant operation and environmental assessment. *Journal of Cleaner Production* 184, 869-892.
- [5] Arbolino, R., Carlucci, F., De Simone, L., Ioppolo, G., Yigitcanlar, T., 2018. The policy diffusion of environmental performance in the European Countries. *Ecological Indicators* 89, 130-138.
- [6] Geissdoerfer, M., Savaget, P., Bocken, N.M., Hultink, E.J. The Circular Economy—A new sustainability paradigm? *Journal of Cleaner Production* 2017, 143, 757-768.
- [7] Moraga, G., Huysveld, S., Mathieu, F., Blengini, G.A., Alaerts, L., Acker, K., Meester, S., Dewulf, J., 2019. Circular economy indicators: What do they measure? *Resources, Conservation and Recycling* 146, 452-461.
- [8] Hysa, E., Kruja, A., Rehman, N.U., Laurenti, R., 2020. Circular economy innovation and environmental sustainability impact on economic growth: An integrated model for sustainable development. *Sustainability* 12(12),4831
- [9] Ingrao, C., Failla, S., Arcidiacono, C., 2020. A comprehensive review of environmental and operational issues of constructed wetland systems. *Current Opinion in Environmental Science and Health* 13, 35-45.
- [10] CE Action plan, 2020. https://ec.europa.eu/environment/circular-economy/pdf/new_circular_economy_action_plan.pdf. Last accessed: March, 2021
- [11] EU, 2019. https://ec.europa.eu/environment/circular-economy/pdf/sustainable_products_circular_economy.pdf. Last accessed: March, 2021
- [12] Chemical Substances, 2011. Chemicals and our environment. Available at: http://www.chemicalsubstanceschimiques.gc.ca/fact-fait/chem-chim_environ-eng.php. Last accessed: December, 2019).
- [13] PlasticsEurope. 2020. <https://www.plasticseurope.org/en> Last accessed: January, 2021
- [14] Tournier, V., Topham, C. M., Gilles A., David, B., Folgoas, C., Moya-Leclair, E., Kamionka, E., Desrousseaux, M.-L., Texier, H., Gavalda, S., Cot, M., Guémard, E., Dalibey, M., Nomme, J., Cioci, G., Barbe, S., Chateau, M., André, I., Duquesne S., Marty, A. 2020. An engineered PET depolymerase to break down and recycle plastic bottles. *Nature* 580(7802), 216-219.
- [15] Al-Salem, S., Lettieri, P., Baeyens, J. 2009. Recycling and recovery routes of plastic solid waste (PSW): a review. *Waste Manage.* 29, 2625-2643
- [16] Zhang, X., Zhang, W., Xie, J., Zhang, C., Fu, J., Zhao, P. 2021. Automatic magnetic projection for one-step separation of mixed plastics using ring magnets . *Science of the Total Environment*. 786,147217
- [17] Scheirs, J. 1998. *Polymer Recycling: Science, Technology, and Applications*. Wiley Series in Polymer Science.
- [18] George, N., Kurian T. 2014. Recent developments in the chemical recycling of postconsumer poly(ethylene terephthalate) waste. *Ind. Eng. Chem. Res.*, 53, 14185-14198
- [19] Barnard, E., Rubio Arias, J.J., Thielemans, W. 2021. Chemolytic depolymerisation of PET: A review. *Green Chemistry*. 23(11), 3765-3789
- [20] Goto M. 2009. Chemical recycling of plastics using sub- and supercritical fluids. *J. Supercrit. Fluids*, 47, 500-507
- [21] Oliveux, G., Bailleul, J.L., La Salle E.L. 2012. Chemical recycling of glass fibre reinforced composites using subcritical water. *Compos. Part A-Appl. Sci.*, 43, 1809-1818
- [22] Sagong, H.-Y., Son, H.F., Seo, H., Hong, H., Lee, D., Kim, K.-J. 2021. Implications for the PET decomposition mechanism through similarity and dissimilarity between PETases from *Rhizobacter gummiphilus* and *Ideonella sakaiensis*. *Journal of Hazardous Materials*. 416,126075
- [23] Ingrao, C., Lo Giudice, A., Tricase, C., Rana, R., Mbohwa, C., Siracusa, V. 2014. Recycled-PET fibre based panels for building thermal insulation: Environmental impact and improvement potential assessment for a greener production. *Science of the Total Environment*. 493, 914-929
- [24] da Silva, T.R., de Azevedo, A.R.G., Cecchin, D., Marvila, M. T., Amran, M., Fediuk, R., Vatin, N., Karelina, M., Klyuev, S., Szelag, M., 2021. Application of plastic wastes in construction materials: A review using the concept of life-cycle assessment in the context of recent research for future perspectives. *Materials*. 14(13),3549
- [25] Ali, S.S., Elsamahy, T., Koutra, E., Zhu, D., Sun, J. 2021. Degradation of conventional plastic wastes in the environment: A review on current status of knowledge and future perspectives of disposal. *Science of the Total Environment*. 771,144719
- [26] Basuhi, R., Moore, E., Gregory, J., Gesing, A., Olivetti, E.A. 202. Environmental and economic implications of U.S. postconsumer plastic waste management. *Resources, Conservation and Recycling*. 167,105391

[26] Bakshi, B.R.2002. A thermodynamic Framework for Ecologically Conscious ProcessSystems Engineering. *Computers & Chemical Engineering* 26(2), 269–282.

[27] Yao, D., Yang, H., Hu, Q., Chen, Y., Chen, H., Williams, P.T., 2021. Carbon nanotubes from post-consumer waste plastics: Investigations into catalyst metal and support material characteristics. *Applied Catalysis B: Environmental* 280, 119413.

[28] Falcone, Pasquale Marcello and Enrica Imbert. 2019. "Tackling Uncertainty in the Bio-Based Economy." *IJSR.17* (1): 74-84

[29] Majer, S.; Wurster, S.; Moosmann, D.; Ladu, L.; Sumfleth, B.; Thrän, D. 2018. Gaps and Research Demand for Sustainability Certification and Standardisation in a Sustainable Bio-Based Economy in the EU. *Sustainability*, 10: 2455.

[30] Bishop, G., Styles, D., Lens, P.N.L. 2021. Environmental performance comparison of bioplastics and petrochemical plastics: A review of life cycle assessment (LCA) methodological decisions. *Resources, Conservation and Recycling*. 168,105451

[31] Schwarz, A.E., Lighthart, T.N., Godoi Bizarro, D., Vreugdenhil, B., van Harmelen, T. 2021. Plastic recycling in a circular economy; determining environmental performance through an LCA matrix model approach. *Waste Management*. 121, 331-342

[32] Plastics-recyclers-europe, 2020. <https://plastics-recyclers-europe.prezly.com/closing-the-loop-with-pet-bottle-to-bottle-recycling-projected-to-grow>. Last accessed: December, 2019.

[33] PlasticsEurope. 2019a. Eco-profiles and Environmental Product Declarations of the Eu-ropean Plastics Manufacturers – Polyethylene Terephthalate (PET) Bottle-Grade.Tech. rep. Last accessed: January, 2021

[34] González-Castaño, A., Bandoni, J.A., Diaz, M.S. 2016. Multi-Objective Optimisation in a Petrochemical Complex with LCA considerations . *Computer Aided Chemical Engineering*. 38, 1497-1502

[35] Zandkarimkhani, S., Nasiri, M.M., Heydari, J. 2020. Sustainable open-loop supply chain network design considering location routing problem: A hybrid approach based on FAHP, FTOPSIS, and mathematical programming. *International Journal of Logistics Systems and Management*. 36(1), 92-123

[36] Winans, K.S., Macadam-Somer, I., Kendall, A., Geyer, R., Marvinney, E. 2020. Life cycle assessment of California unsweetened almond milk. *International Journal of Life Cycle Assessment*. 25(3), 577-587

[37] Błażejewski, T., Walker, S.R., Muazu, R.I., Rothman, R.H. 2021. Reimagining the milk supply chain: Reusable vessels for bulk delivery *Sustainable Production and Consumption*. 27, 1030-1046

[38] Odum, H.T. 1996. *Environmental Accounting: Emergy and Environmental Decision Making*. John Wiley & Sons, New York

[39] Pulselli FM, Patrizi N, Focardi S. Calculation of the unit energy value of water in an Italian watershed. *Ecol Model* 2011;222:2929–38.

[40] Bastianoni, S., Campbell, D., Susani, L., Tiezzi, E. 2005. The Solar Transformity of Oil and Petroleum Natural Gas. *Ecological Modelling* 86, 212–220

[41] Bastianoni, S., Campbell, D.E., Ridolfi, R., Pulselli, F.M. 2009. The Solar Transformity of Petroleum Fuels. *Ecological Modelling* 220, 40–50

[42] Sha Sha, Melin, K., Villalba de Kokkonen, D., Hurme, M. 2015. Solar Energy Footprint of Ethylene Processes. *Ecological Engineering* 82, 15–25

[43] Brown, M.T., Protano, G., Ulgiati, S. 2011. Assessing geobiosphere work of generating global reserves of coal, crude oil, and natural gas. *Ecological Modelling*. 222(3), 879-887

[44] Bakshi BR. A thermodynamic framework for ecologically conscious process systems engineering. *Comput Chem Eng* 2000;24:1767–73.

[45] Marvuglia A, Santagata R, Rugani B, Benetto E, Ulgiati S. Emergy-based indicators to measure circularity: promises and problems. *Polityka Energetyczna* 2018;21.

[46] Marvuglia A, Benetto E, Rios G, Rugani B. SCALE: software for CALCulating Emergy based on life cycle inventories. *Ecol Model* 2013;248:80–91.

[47] Arbault D, Rugani B, Marvuglia A, Benetto E, Tiruta-Barna L. Emergy evaluation using the calculation software SCALE: case study, added value and potential improvements. *Sci Total Environ* 2014;472:608–19.

[48] Raugei M, Rugani B, Benetto E, Ingwersen WW. Integrating emergy into LCA: potential added value and lingering obstacles. *Ecol Model* 2014;271:4–9.

[49] Hau JL, Bakshi BR. Promise and problems of emergy analysis. *Ecol Model* 2004; 178:215–25.

[50] Santagata R, Zucaro A, Fiorentino G, Lucagnano E, Ulgiati S. 2020. Developing a procedure for the integration of life cycle assessment and emergy accounting approaches. The Amalfi paper case study. *Ecological Indicators*. 117:106676.

[51] Whitesides, G.M., 2015. Reinventing chemistry. *Angewandte Chemie - International Edition* 54(11), 3196-3209.

[52] Almeida, C. M.V.B., Rodrigues, A., Bonilla, S., Giannetti, B.F. 2010. Emergy as a Tool for Ecodesign: Evaluating Materials Selection for Beverage Packages in Brazil. *Journal of Cleaner Production* 18(1), 32–43

[53] Almeida, C.M.V.B., Rodrigues, A.J.M., Agostinho, F., Giannetti, B.F. 2017. Material selection for environmental responsibility: the case of soft drinks packaging in Brazil. *Journal of Cleaner Production*. 142, 173-179

[54] Bustamante, G., Giannetti, B.F., Agostinho, F., de Silva, M.T., Almeida, C.M.V.B. 2016 *IFIP Advances in Information and Communication Technology* 488, 812-827

[55] ISO (International Organization for Standardization). 14040-Environmental management - Life cycle assessment - Principles and framework. 2006a. <https://www.iso.org/standard/37456.html>.

[56] ISO (International Organization for Standardization). 14044-Environmental management - Life cycle assessment - Requirements and guidelines. 2006b. <https://www.iso.org/standard/38498.html>.

[57] PlasticsEurope. 2019b. Plastics—the facts 2019. An analysis of European plastics production, demand and waste data. PlasticsEurope
https://www.plasticseurope.org/application/files/1115/7236/4388/FINAL_web_version_Plastics_the_facts2019_14102019.pdf. Last accessed: January, 2021

[58] Brown MT, Herendeen RA. Embodied energy analysis and EMERGY analysis: a comparative view. *Ecol Econ* 1996;19:219–35.

[59] Herendeen R. Embodied energy, embodied everything... Now what. *Advances in energy studies. Energy flows in ecology and economy* 1998;13–48.

[60] Slesser M. Energy analysis workshop on methodology and conventions, vol. 89. Stockholm, Sweden: IFIAS; 1974.

[61] Brown, M.T., Campbell, D.E., De Vilbiss, C., Ulgiati, S. 2016. The geobiosphere energy baseline: a synthesis. *Ecological Modelling* 339, 92-95

[62] Li-Na, J. 2013. Study on preparation process and properties of polyethylene terephthalate (PET). *Appl Mech Mater* 312:406–410.

[63] Yue, H., Zhao, Y., Ma, X., Gong, J. 2012. Ethylene glycol: properties, synthesis, and applications. *Chem Soc Rev* 41:4218–4244.

[64] Lyu Y, Raugei M, Zhang X, Mellino S, Ulgiati S. 2021 Environmental cost and impacts of chemicals used in agriculture: An integration of emergy and Life Cycle Assessment. *Renewable and Sustainable Energy Reviews* 151: 111604

[65] Ulgiati S, Brown MT. 2014 Labor and services as information carriers in Emergy-LCA accounting. *Journal of Environmental Accounting and Management*. 2: 163–70.

[66] Giannetti, B.F., Marcilio, M.F.D.F.B., Coscieme, L. Agostinho, F., Liu, G., Almeida,C.M.V.B., 2019a. Howard Odum's "Self-organization, transformity and information": Three decades of empirical evidence. *Ecological Modelling*. 407,108717

[67] Laville, S., Taylor, M. 2021. A million bottles a minute: world's plastic binge 'as dangerous as climate change. *The Guardian*, 28 Jun 2017. Last accessed: January, 2021

[68] Cleary, J. 2013. Life cycle assessments of wine and spirit packaging at the product and the municipal scale: a Toronto, Canada case study. *J. Clean. Prod.*, 44, 143-151

[69] Santos, R., Silva, É.F.M., Dantas, E.J.M., Garcia, R.R.P., Almeida, L.C. 2020. Potential Reuse of PET Waste Bottles as a Green Substrate/Adsorbent for Reactive Black 5 Dye Removal. *Water, Air, and Soil Pollution*. 231(11),533

[70] Giannetti, B.F., Bonilla, S.H., Almeida, C.M.V.B. 2004. Developing eco-technologies, a possibility to minimize environmental impact in Southern Brazil. *J. Clean. Prod.*, 12, 361-368

[71] Xu, X. Zhou, Z. Lei, K. LeBlanc, G.A., Na, L. 2019 . Phthalate Esters and Their Potential Risk in PET Bottled Water Stored under Common Conditions. *Int J Environ Res Public Health*. 17(1):141.

[72] Pang, J., Zheng, M., Sun, R., Wang, A., Wang, X., Zhang, T. 2016. Synthesis of ethylene glycol and terephthalic acid from biomass for producing PET. *Green Chem* 18:342–359.

[73] Dutta, S., Bhat, N.S. 2020. Catalytic synthesis of renewable p-xylene from biomass-derived 2,5-dimethylfuran: a mini review. *Biomass Conversion and Biorefinery*. Published online 03 October 2020

[74] Coca-cola, 2009. <https://www.coca-colacompany.com/faqs/what-is-plantbottle-packaging>. Last accessed: January, 2021

[75] BBC, 2021 https://www.bbc.com/news/technology-56023723?fbclid=IwAR1wo7ef9q5HeI0KEZ5CJtW4Jbv0fX_ILpXwBmGBtCyMABCJ5qaItOXuFY. Last accessed: January, 2021

[76] Bleischwitz, R., Spataru, C., VanDeveer, S.D., Obersteiner, M., van der Voet, E., Johnson, C., Andrews-Speed, P., Boersma, T., Hoff, H., van Vuuren, D.P., 2018. Resource nexus perspectives towards the United Nations Sustainable Development Goals. *Nat Sustain* 1, 737–743. <https://doi.org/10.1038/s41893-018-0173-2>

[77] Palacios-Mateo, C., van der Meer, Y., Seide, G. 2021. Analysis of the polyester clothing value chain to identify key intervention points for sustainability. *Environmental Sciences Europe* 33(1), 2.

[78] Hacini, M., Benosman, A.S., Kazi Tani, N., Badache, A., Latroch, N. 2021. Utilization and assessment of recycled polyethylene terephthalate strapping bands as lightweight aggregates in Eco-efficient composite mortars. *Construction and Building Materials*. 270,121427

[79] Martin, E.J.P., Oliveira, D.S.B.L., Oliveira, L.S.B.L., Bezerra, B.S. 2021. Life cycle comparative assessment of pet bottle waste management options: A case study for the city of Bauru, Brazil. *Waste Management*. 119, 226-234

[80] Di, J., Reck, B.K., Miatto, A., Graedel, T.E. 2021. United States plastics: Large flows, short lifetimes, and negligible recycling. *Resources, Conservation and Recycling*. 167,105440

[81] Giannetti, B.F., Sevegnani, F., Almeida, C.M.V.B., Agostinho, F., Moreno García, R.R., Liu, G. 2019b. Five sector sustainability model: A proposal for assessing sustainability of production systems. *Ecological Modelling*. 406, 98-108