ANL/ESIA-24/3

Life-Cycle Analysis Datasets for Regionalized Plastic Pathways

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Energy Systems and Infrastructure Analysis Division

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Abbreviations and Acronyms

ANL	Argonne National Laboratory
C_2H_2	Acetylene
C_2H_4	Ethylene
C_3H_6	Propylene
CaC_2	Calcium carbide
CEH	Chemical Economics Handbook
CH_4	Methane
CI	Carbon intensity
Cl_2	Chloride
CO_2	Carbon dioxide
DMT	Dimethyl terephthalate
DOE	Department of Energy
EDC	Ethylene dichloride
EG	Ethylene glycol
FCC	Fluid catalytic cracking
GHG	Greenhouse gas
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation
GWP	Global warming potential
H_2	Hydrogen
HCl	Hydrochloric acid
HDPE	High-density polyethylene
IPCC	Intergovernmental Panel on Climate Change
LCA	Life cycle analysis
LCI	Life cycle inventory
LDPE	Low-density polyethylene
MENA	Middle East and North Africa
MMT	Million metric tonnes
N_2O	Nitrous oxide
NaCl	Sodium chloride
NaOH	Sodium hydroxide
NG	Natural gas
NGL	Natural gas liquids
NIST	National Institute of Standards and Technology
OECD	Organisation for Economic Cooperation and Development
PDH	Propane dehydrogenation
PE	Polyethylene

PET	Polyethylene terephthalate
PP	Polypropylene
PTA	Purified terephthalic acid
PVC	Polyvinyl chloride
USA	United States of America
VCM	Vinyl chloride monomer

Acknowledgments

This work was supported by the National Institute of Standards and Technology (NIST) under proposal number P22-730-0003. However, the opinions and conclusions presented herein are exclusively those of the authors. We sincerely appreciate all input, review and feedback provided by David Butry, David Webb, and Noah Last at NIST. We also appreciate Ulises R. Gracida-Alvarez for helping with the literature review and Pradeep Vyawahare at Argonne National Laboratory for providing advice on the chlor-alkali process in the United States.

Executive Summary

The carbon intensity (CI) of producing five different resins – polyethylene terephthalate (PET), high-density polyethylene (HDPE), low-density polyethylene (LDPE), polypropylene (PP), and polyvinyl chloride (PVC) – in four different regions – United States of America (USA), Western Europe, Middle East and Northern Africa (MENA), and China – is calculated on a cradle-to-gate basis using the Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) model.[1] In this research, some of the important potential factors affecting the CI of the five resins in different regions are identified. These factors include the CI of electricity and natural gas (NG) production, steam cracking feedstock mix, propylene sourcing technology mix, terephthalic monomer mix, use of hydrogen co-product from steam cracking process, and vinyl chloride monomer (VCM) production technology mix.

The GHG emissions results are presented for each of the four regions. An example of the cross-regional CI results is shown in Figure 1. The CI of PET resin produced in the four regions is presented in Figure 1-(a) while the contributions from each process to cross-regional variations in CI is presented in Figure 1-(b). In Figure 1-(a), we can compare each of the regions' CI of PET to the average CI across the four regions (1.91 $kgCO_2e/kg$-PET). The figure also presents the variables that contribute to the regional variations in the CI of PET: dimethyl terephthalate (DMT) monomer shares in PET polymerization and the NG liquid (NGL) share in the steam cracking feedstock mix. The cradle-to-gate GHG emissions results for each of the five resins are presented in a similar figure style to identify the quantitative differences in the CI across the regions and the main causes for those differences.

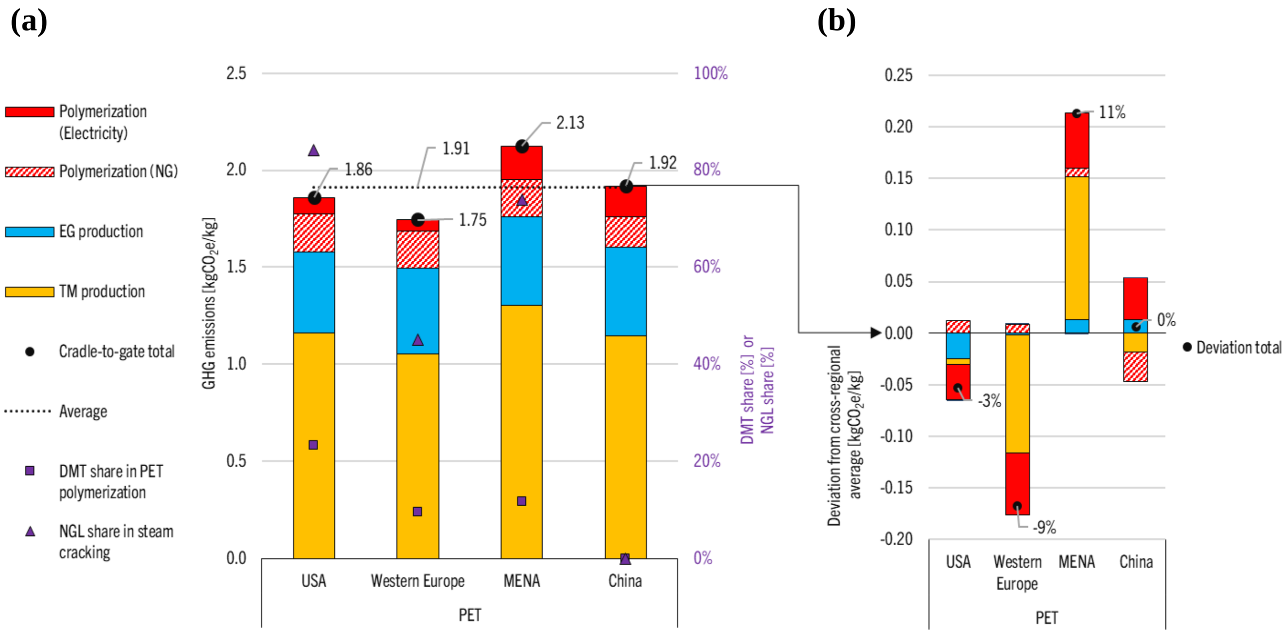

Figure 1. (a) Cradle-to-gate GHG emissions results for PET in four different regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average.

Table 1 presents the summary of results for the five resins' CI across the four regions. PET, LDPE, HDPE, and PP showed a moderate degree of cross-regional variations in CI, which ranged around or within ±10% deviation from each of their cross-regional average CI. However, PVC showed significant cross-regional variations in CI: approximately 17% lower CI and 34% higher CI in Western Europe and China, respectively, compared to the cross-regional average CI. For all five resins, the regional variation in the CI of electricity was one of the most important factors. Electricity in the USA and Western Europe had a lower CI compared to MENA and China, thus resulting in a lower CI of resins compared to that produced in MENA and China. The importance of the CI of electricity and other energy resources required to produce resin has been reported in a previous study.[2] Cabernard et al.[2] reported that the carbon footprint of global resin production has doubled between 1995 and 2015, which was mainly due to the increase in resin production using coal-based electricity and other energy resources in some countries and economies.

Table 1: Summary of key results for the five resins' cross-regional CI.

		PET	HDPE	LDPE	PP	PVC
Cross-regional average [kgCO$_2$e/kg]		1.91	1.42	1.81	1.25	2.68
Regions with the lowest and highest CI	1st (Min. CI)	Western Europe (-9%)*	USA (-7%)*	Western Europe (-9%)*	USA (-8%)*	Western Europe (-17%)*
	2nd	USA (-3%)*	Western Europe (-5%)*	USA (-8%)*	Western Europe (2%)*	USA (-16%)*
	3rd	China (0%)*	MENA (4%)*	China (8%)*	MENA (2%)*	MENA (-1%)*
	4th (Max. CI)	MENA (11%)*	China (7%)*	MENA (9%)*	China (3%)*	China (34%)*
Key contributors for cross-regional variations		CI of electricity	CI of electricity	CI of electricity	CI of electricity	CI of electricity
			Steam cracking feedstock mix	Steam cracking feedstock mix	Steam cracking feedstock mix	VCM technology mix
					Propylene sourcing mix	
Minor contributors for cross-regional variations		CI of NG production	CI of NG production	CI of NG production	CI of NG production	CI of NG production
		Steam cracking feedstock mix				Steam cracking feedstock mix
		Terephthalic monomer mix				

*Note: Percentages in the parentheses mean the % deviation from the cross-regional average CI.

For polyolefins (i.e., HDPE, LDPE, and PP), the regional variation in the steam cracking feedstock mix was another key contributor to regional variation in the CI of polyolefins. Those regions with higher NGL share in their steam cracking feedstock mix had relatively lower CI of polyolefins compared to regions with higher petroleum share. This is consistent with the trend reported by Hermann et al.[3] They reported that the CI of olefin tends to be more carbon-intensive in the regions leveraging more coal- or petroleum-based feedstocks for olefin production that, in turn, resulted in more carbon-intensive polyolefins than using NG-based feedstocks.[3] For PP, regional variation in the propylene sourcing mix was also an important contributor. Those regions with higher non-steam cracking propylene sourcing had relatively lower CI than the regions with higher steam cracking propylene sourcing mix.

For PVC, regional variation in the VCM production technology mix was another important factor contributing to different energy consumption in the PVC's supply chain, thus resulting in different cradle-to-gate CI of PVC in four regions. China had significantly higher CI for PVC production due to the high reliance on acetylene-based VCM compared to the other regions.

1. Introduction

Plastic's numerous applications have made the material an indispensable part of modern civilization. However, plastic production has significant impacts on our environment. According to the Organization for Economic Co-operation and Development (OECD), plastic production is responsible for approximately 3-4% of global greenhouse gas (GHG) emissions. This is comparable to the contributions from the global aviation or maritime sector.[4] Although there has been much previous research on the life cycle GHG emissions of plastics, the research regarding the plastics' carbon intensity (CI) across different global regions is relatively sparce. This has left some important gaps to be addressed in the life cycle analysis (LCA) of plastics because the location of resin production can potentially impact the CI of resin significantly due to multiple factors that can vary across different regions. For example, a recent study on the CI variation of propylene shows that the CI can vary by an order of magnitude depending on its region of production.[3]

Addressing the differences in the CI of major resins produced in different regions will help reduce the uncertainty of the CI of major resins through investigation in their supply chains.

In this study, five major resins' CI in four different regions of production is investigated. Using the current version of the GREET model[1] in conjunction with international electricity and natural gas (NG) production datasets, the CI of resins specific to each region is estimated. The detailed description on the electricity generation and NG production for regions used for this study is provided in Section 2.5. The cross-regional average is compared to the CI of each resin in each region. Contributions from different resin production processes and material/energy inputs on the GHG emissions are compared across different regions to gain knowledge on the source of cross-regional variations in the CI of resins. Sensitivity analyses are also conducted with a range of hydrogen combustion rate in steam crackers since it could potentially cause regional variations in the resins' CI.

2. Methods and Approach

2.1. Choice of resins

Through a literature review, five resins with the highest annual production volume were selected: polyethylene terephthalate (PET), high-density polyethylene (HDPE), low-density polyethylene (LDPE), polypropylene (PP), and polyvinyl chloride (PVC). These resins are consistently identified as the top five resins globally by production volume.[5-7] Table 2 shows a summary of production volume shares and annual consumption volume for different resin types reported in other literatures. Geyer et al.[5] presents the share for each of the five resins in global plastic production volume for 2015, and PP (21%) accounted for the highest ratio out of the total plastic production followed by the LDPE (20%), HDPE (16%), PVC (12%), and then by the PET (10%). Polystyrene (PS) accounted for about 8% of total worldwide plastic production while all other plastics (polycarbonate, polyurethane, etc.) combined accounted for only 13% of the total plastic production. Nicholson et al.[6] also reports the abovementioned five resins as the most produced and consumed resins globally around the timeframe of 2019: all PEs [92.9 million metric tonne (MMT)/yr] followed by PET (62.3 MMT/yr), PP (52.6 MMT/yr), and then by PVC (45.6 MMT/yr). In Nicholson's study[6], PET for textile purposes were included in PET resin production, thus resulting in the 2nd most produced resin while the study conducted by Geyer et al.[5] did not include that portion of PET in the statistics. However, the fact that PET, HDPE, LDPE, PP, and PVC were the top five most produced and consumed resins worldwide was consistent between the two literatures.

Table 2: Share of production volume and annual consumption volume of different resins based on previous publication

Resin type	Share of production volume out of global plastic production (based on Geyer et al.[5])	Annual global consumption volume [MMT/yr] (based on Nicolson et al.[6])
PP	21%	52.6
LDPE	20%	92.9 (all PEs)
HDPE	16%	
PVC	12%	45.6
PET	10% (excluding PET for textile)	62.3 (including PET for textile)
PS	8%	28.5

Finally, we collected annual production volume for each of these five resins from the Chemical Economics Handbook (CEH) marketing research reports: PET[8], HDPE[9], LDPE[10], PP[11], and PVC[12], which is presented in

Table 3.

Table 3: Global annual production volume for each of the five resins investigated in this study (Based on CEH marketing research report in the timeframe of 2010-2012).

	PET[8]	HDPE[9]	LDPE[10]	PP[11]	PVC[12]
Global annual production volume [MMT/yr]	56.3	32.0	18.6	48.8	35.4

2.2. Choice of regions

The regions that accounted for most production of the selected five resins are identified, with four regions being selected. Figure 2 shows the list of those four regions: i) United States of America (USA); ii) Western Europe; iii) Middle East and North Africa (MENA); and iv) China. These four regions combined accounted for approximately two-thirds of the global production volume for each of the five resins. The production volume for each region regarding each resin is referenced from the CEH marketing research report: PET[8], HDPE[9], LDPE[10], PP[11], and PVC,[12] and is summarized in Figure 2.

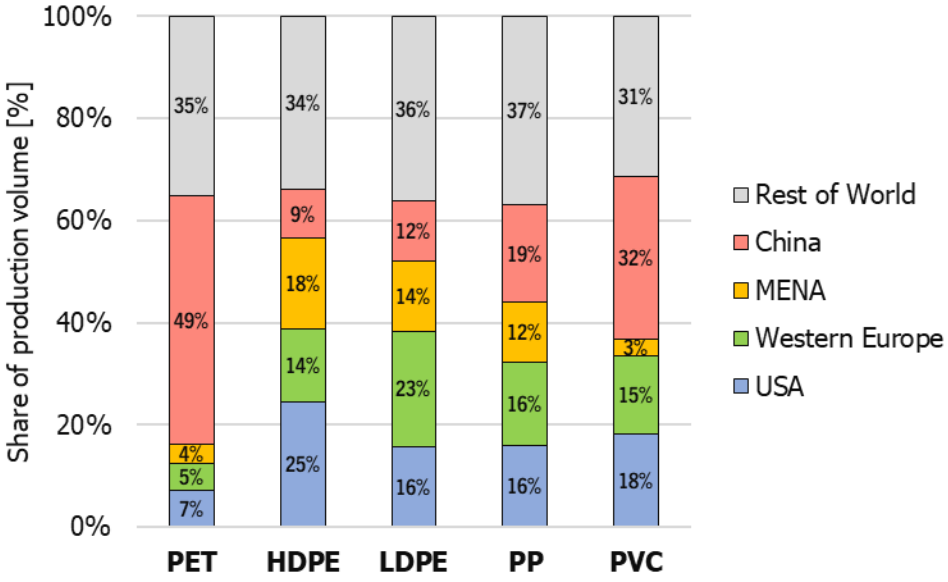

Figure 2. Regional share of resin production

2.3. System boundary

2.3.1. Polyethylene terephthalate (PET)

Figure 3 shows the system boundary for PET production. PET is produced from the polymerization of two different monomers, or namely the ethylene glycol (EG) monomer and terephthalic monomer.[13] In this study, EG is assumed to be produced through a conventional pathway where different fossil-fuel feedstocks (i.e., natural gas liquids (NGL) and petroleum) are used to first produce ethylene (C_2H_4) via steam cracking,[14] and then ethylene-to-EG conversion via oxidation of ethylene-to-ethylene oxide followed by hydrolysis of ethylene oxide-to-EG. For terephthalic monomer, there are two different types that are currently used to produce PET: i) purified terephthalic acid (PTA); and ii) dimethyl terephthalate (DMT). Both terephthalic monomers are produced from the oxidation of p-xylene sourced from the benzene-toluene-xylene (BTX) stream of the petroleum refinery.[15]

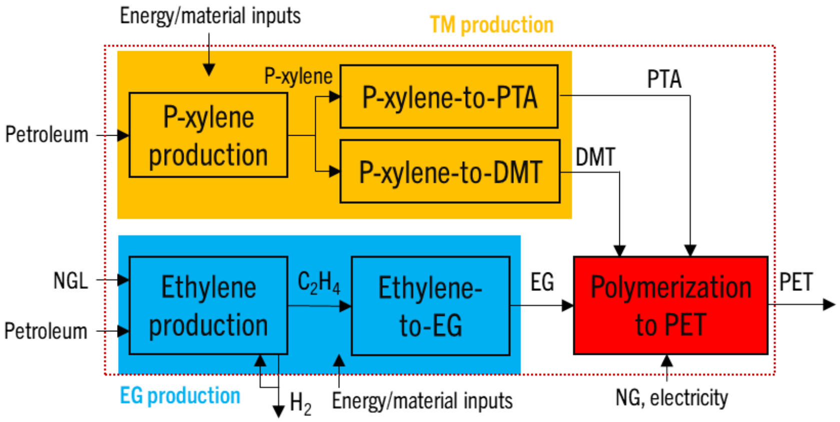

Figure 3. Process flows and system boundary (red dashed line) for PET production. The processes are marked with the same color-code used in Figure 16.

2.3.2. High-Density Polyethylene (HDPE)

Figure 4 shows the system boundary for HDPE production. HDPE is produced from the polymerization of ethylene sourced from steam cracking of two different fossil-fuel feedstocks (i.e., NGL and petroleum).[13,16] During the steam cracking process, other olefins (e.g., propylene, butylene) and chemical products (e.g., hydrogen, butadiene) are co-produced.[17] Some of the hydrogen co-produced in the steam cracking process is assumed to be combusted for thermal energy recovery purposes. More details on the assumptions made on the steam cracking process are presented in Section 2.5.2.

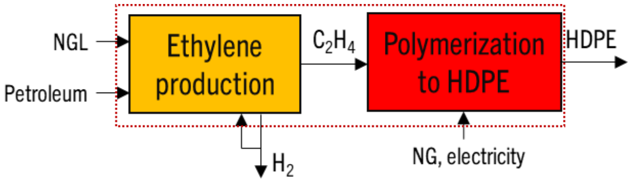

Figure 4. Process flows and system boundary (red dashed line) for HDPE production. The processes are marked with the same color-code used in Figure 20.

2.3.3. Low-Density Polyethylene (LDPE)

Figure 5 shows the system boundary for LDPE production. LDPE production is similar to HDPE except for some details regarding its polymerization process. Typically, the polymerization process required for LDPE consumes more thermal and electrical energy compared to that required for HDPE.[18,19] In the GREET model, while the HDPE polymerization process is estimated to consume 1.62 MJ of NG and 1.11 MJ of electricity per kg production of HDPE, the LDPE polymerization process is estimated to consume 4.07 MJ of NG and 2.44 MJ of electricity per kg production of LDPE.[1] This difference in energy consumption is mainly due to the difference in the reactor types between the two polymerization technologies used for HDPE and LDPE: HDPE polymerization uses low-pressure reactor while the LDPE polymerization uses high-pressure reactor requiring more energy.[16,18]

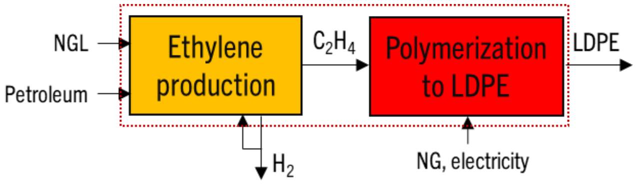

Figure 5. Process flows and system boundary (red dashed line) for LDPE production. The processes are marked with the same color-code used in Figure 21.

2.3.4. Polypropylene (PP)

Figure 6 shows the system boundary for PP production. PP is produced through the polymerization of propylene (C_3H_6) sourced from three main technological pathways: i) steam cracking; ii) fluid catalytic cracking (FCC); and iii) propane dehydrogenation (PDH).[11,13] The steam cracking process often produces propylene as a co-product of ethylene.[17] FCC is another mainstream propylene production pathway where the propylene is co-produced with gasoline and distillate, main products from the cracking of heavy oils.[11] Although relatively less common, the PDH pathway also produces a noticeable share of propylene. In the PDH pathway, propane is dehydrogenated through a catalyst over 500 °C temperature condition.[11]

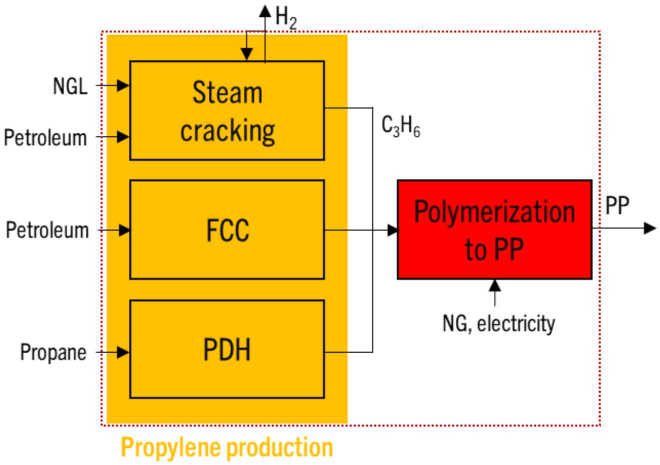

Figure 6. Process flows and system boundary (red dashed line) for PP production. The processes are marked with the same color-code used in Figure 22.

2.3.5. Polyvinyl Chloride (PVC)

Figure 7 shows the system boundary of PVC production. PVC is produced via polymerization of its monomer, or namely the vinyl chloride monomer (VCM).[12] And the VCM can be produced in two different technological pathways: i) acetylene-based VCM production; and ii) ethylene dichloride (EDC)-based VCM production.[20] For the acetylene (C_2H_2)-based VCM pathway, the VCM is prepared through the reaction of acetylene and hydrochloric acid (HCl), and acetylene and hydrochloric acid are produced from coal and sodium chloride (NaCl), respectively.[12] For the EDC-based VCM pathway, VCM is prepared through the reaction of ethylene and chlorine (Cl_2) (or sometimes HCl). Ethylene is sourced from the steam cracking process while Cl_2 (or HCl) is sourced from the chlor-alkali process that electrolyzes NaCl into Cl_2, NaOH, and H_2.[12] Since the acetylene is sourced from calcium carbide (CaC_2) which is derived from coal[12], the CI of acetylene-based VCM production is higher than that of EDC-based VCM production.

Unlike the other four resins presented in the previous sections, the PVC pathway in the current version of GREET has the life-cycle inventory (LCI) for the PVC pathway on a cradle-to-gate basis, not on a unit process level basis.[21] To avoid any confusion for the readers, unlike the Figure 3 – Figure 6, color codes are not used in Figure 7 to represent certain breakdown categories used in its cradle-to-gate GHG emissions result (Figure 24). Instead, a light green dashed line is drawn to distinguish the acetylene-based VCM pathway from the EDC-based VCM pathway.

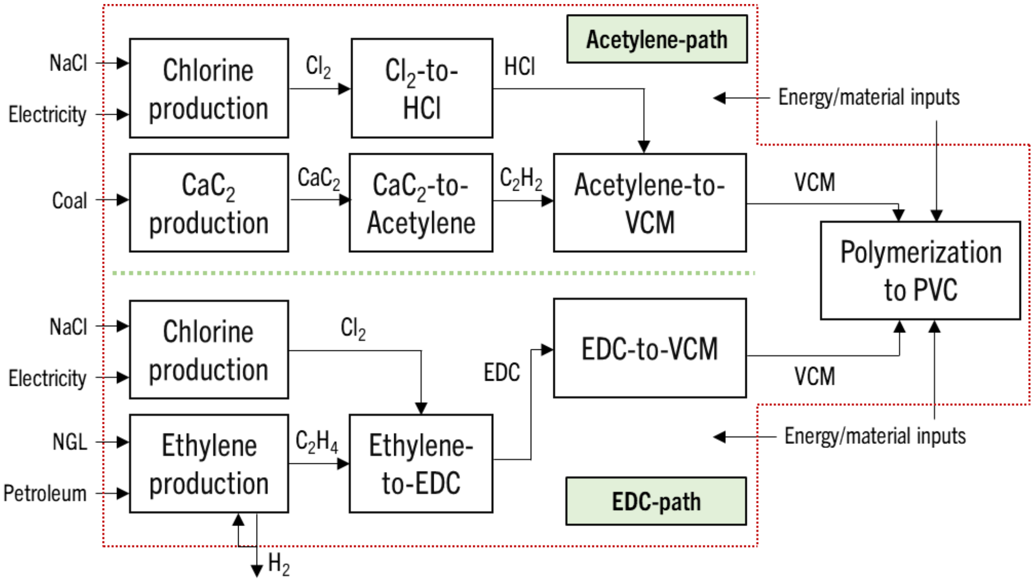

Figure 7. Process flows and system boundary (red dashed line) for PVC production.

2.4. Functional unit and LCA metrics

In this study, the GHG emissions to produce five resins in four regions are calculated in the functional unit of “per kg” on a cradle-to-gate basis. For the global warming potential (GWP), the 100-year GWP defined in Intergovernmental Panel on Climate Change (IPCC)’s 6th Assessment Report (AR6)[22] is used: 1 for CO_2; 29.8 for CH_4; and 273 for N_2O.

2.5. Approach, data sources, and assumptions for baseline analysis

Table 4 shows the summary of the factors that can potentially vary the CI of resins across the four regions. “Y” (Yes) in each cell means that the factor listed on the left-most column can potentially affect the CI of the corresponding resin while “N” (No) in each cell means that the factor is will not affect the CI of the corresponding resin.

To address the differences in the CI of electricity and NG production in different regions, the GREET 2022 model[1] was modified and configured with the region-specific data to derive upstream GHG emission intensities of electricity and NG for the regions of China, EU, and MENA in 2020. The method is similar to the configuration used for the China-GREET model described in Gan et al.[23] For the electricity generation, the key parameters include regional electricity generation mixes, thermal efficiencies of coal-, oil-, gas-, and biomass-fired power plants, electricity transmission and distribution loss rates, and on-site CO_2, CH_4, and N_2O emissions from thermal power plants by fuel type. Relevant data were collected and processed from different International Energy Agency (IEA) statistics, including World Energy Statistics and Balance[24], Electricity Information[25], and Greenhouse Gas Emissions from Energy.[26] For the NG production, we rely on an expansion of our previous work about the engineering-based LCA modelling of hundreds of gas fields in 36 countries, which together covered about 90% of the global NG production in 2020.[27] The parameters configured include regional energy efficiencies and processing fuel shares for both NG recovery and processing, and energy efficiencies of NG liquefaction and liquified NG (LNG) regasification for LNG-associated gas supplies. The regional CH_4 and CO_2 venting, flaring, and fugitive (VFF) emissions during NG production and transportation were derived from IEA statistics.[26,28] It should be noted that all the above-mentioned parameters in the NG sector are production-based. We further developed detailed global NG transportation networks for both pipeline gas and LNG in 2020 based on IEA Natural Gas Information[29] and converted these regional production-based parameters to the supply-based ones for the model configuration. With the developed global NG transportation networks, the transportation distances for both pipeline gases and LNG shipping were also estimated and updated for the studied regions.

The Chemical Economic Handbook (CEH) marketing research reports were used to collect the regional steam cracking feedstock mixes[30], propylene sourcing technology mixes[31], terephthalic monomer share mix in PET production[8], and VCM production technology mix in PVC production.[12] The GREET model version 2022[1] was used to compute all the CI of the resins investigated in this report based on the input information for each of the regions.

Although the list presented in Table 4 covers many different aspects that can potentially generate cross-regional variations in the resins' CI, it should be noted that this list is not exhaustive and other factors that are not listed in this table also affect the regional CI of resin production. For example, depending on the scenario used to treat co-produced hydrogen (i.e., hydrogen combustion for thermal energy recovery versus including hydrogen in the product basket of a steam cracker) in steam cracking process in each region, the CI of olefins (e.g., ethylene and propylene) can vary across different regions and affect the cradle-to-gate CI of most resins. However, due to the lack of dataset for each of the regions studied, the hydrogen use scenario is assumed identical for all four regions studied.[1,14]

In addition, material and energy consumption for a particular resin production technology were considered consistent across the four regions despite the possibility of regional variation or improvements in the technology. For example, the PTA-based PET production pathway might consume different amounts of electricity and thermal energy in their polymerization process depending on the region of production and different optimized conditions for each specific production plants. However, all regions are assumed to consume the identical amount of electricity (0.23 kWh/kg-PET) and NG (2.27 MJ/kg-PET) for its PTA-based PET pathway.[1] The factor we customized for each region was how much share of PET is produced from each different technological pathway (i.e., PTA-based vs. DMT-based).

Table 4: Summary of the regional datasets that can potentially affect the CI of resins across the four regions.

List of the regional datasets collected in this study	PET	HDPE	LDPE	PP	PVC
Electricity grid mix	Y	Y	Y	Y	Y
NG supply chain	Y	Y	Y	Y	Y
Steam cracking feedstock mix[30] (NGL vs. petroleum)	Y	Y	Y	Y	N
Propylene sources[31] (steam cracking vs. non-steam cracking processes such as FCC and PDH)	N	N	N	Y	N

Terephthalic monomer type for PET production[8] (PTA vs. DMT)	Y	N	N	N	N
Acetylene vs. EDC pathway mix in VCM production[12]	N	N	N	N	Y

Figure 8 presents the structure of the datasets referenced from CEH marketing research reports to collect region-specific characteristics such as steam cracking feedstock mix, propylene sourcing mix, terephthalic monomer mix, and VCM pathway mix. Each region is composed of one or more countries, and each country is composed of one or more production plants. The datasets available in the CEH marketing research reports are granular to the production plant level.[8,12]

Thus, a region-specific characteristic could be calculated from a bottom-up approach using the plant-level data.

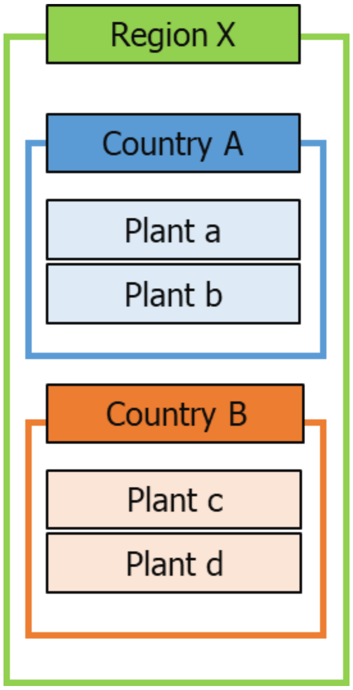

Figure 8. Data structure of the reference datasets to calculate region-specific steam cracking feedstock mix, propylene sourcing mix, terephthalic monomer mix, and VCM pathway mix.

An example of how a region-specific terephthalic monomer mix is calculated using the plant-level datasets collected from the reference is as follows.[8] First, the terephthalic monomer type used for PET production at each production plant is identified with the production capacity of each plant. Then, each country's terephthalic monomer mix is calculated using the plant-level PET production capacity with specified terephthalic monomer type. Then, region's terephthalic monomer mix is calculated using the country-level terephthalic monomer mix. This approach is applied the same for the calculation of other region-specific characteristics such as steam cracking feedstock mix, propylene sourcing mix, and VCM pathway mix.

2.5.1. Polyethylene terephthalate (PET)

For PET, the following four factors are identified to potentially cause the variation in its CI across the regions:

- CI of electricity in the region of resin production;
- CI of NG production in the region of resin production;
- Steam cracking feedstock mix in the region of resin production; and
- DMT- and PTA-path share in each region's PET production pool.

The steam cracking feedstock mix in each region affected the CI of ethylene that, in turn, affected the CI of EG and then PET. Also, due to the different energy and material consumption required for DMT and PTA production, the CI of terephthalic monomer can vary across the region if the pathway share for each terephthalic monomer type is different across the regions.

Figure 9 shows the share of each terephthalic monomer type used for PET production in each region in 2011. In all four regions, the share of DMT-path is much lower than that of PTA-path.[8] Although the USA was estimated to have the highest DMT share in its PET production pool out of the four regions, the ratio was approximately 23%. China was estimated to produce PET only via PTA-pathway. The figure also presents the annual production capacity in each region for comparison purposes. China is the dominant producer of PET globally, followed by the USA, Western Europe, and then MENA.

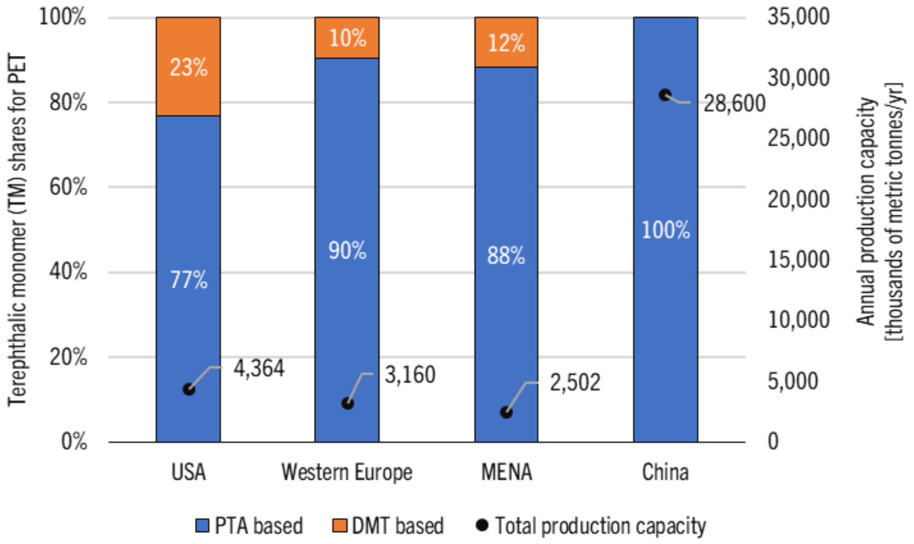

Figure 9. Shares of PTA- and DMT-path for PET production in each region with annual PET production capacity.

2.5.2. Polyolefins (HDPE, LDPE, and PP)

For all three polyolefins, the following factors are identified to potentially cause cross-regional variations in the resins' CI:

- CI of electricity in the region of resin production;
- CI of NG production in the region of resin production; and
- Steam cracking feedstock mix in the region of resin production.

Then, for PP, the differences in the propylene sourcing pathway mix in each region of resin production was also identified as the factor to vary the CI of PP across different regions.

Figure 10 shows the feedstock mix for the steam cracking plants in each region in 2010. In the USA and MENA, NGL was the dominant steam cracking feedstock while, for Western Europe and China, petroleum-based product (e.g., naphtha) was relatively more commonly used as the steam cracking feedstock. The figure also presents the annual production capacity of ethylene in each region for comparison purposes.

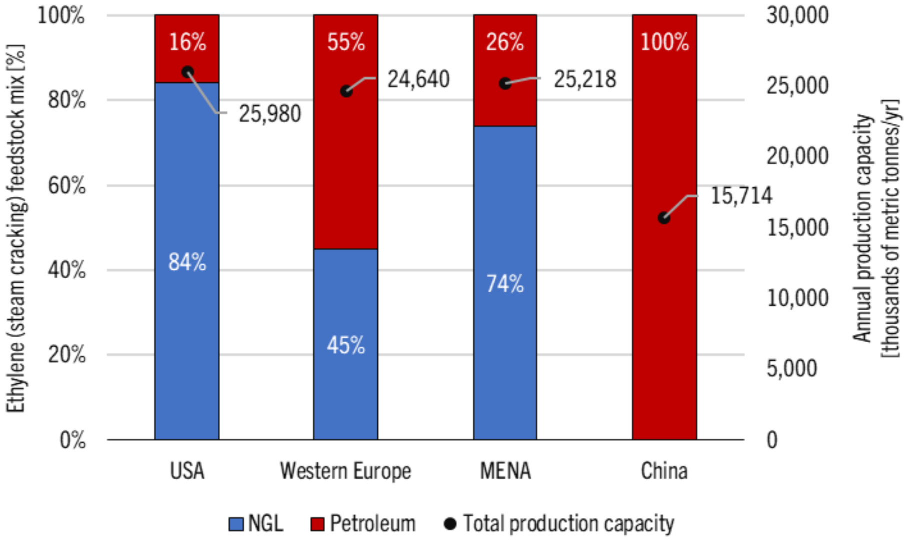

Figure 10. Shares of NGL and petroleum in the steam cracking feedstock mix in each region with annual ethylene production capacity.

Figure 11 shows the technology mix for propylene production in each region in 2011. While steam cracking was more prevalent in Western Europe, different non-steam cracking technologies were more dominant in the USA (i.e., FCC) and MENA (i.e., PDH). In China, steam cracking accounted for approximately half of the propylene production and the rest was produced via non-steam cracking pathways such as FCC and PDH. The figure also presents the annual production capacity of propylene in each region for comparison purposes.

For the olefins produced, there were some important assumptions we made in this study. First, during the steam cracking process, different olefins (e.g., ethylene, propylene, butylene) and chemical products (e.g., hydrogen, butadiene, pyrolysis gasoline, etc.) are co-produced. For the hydrogen co-product, it is assumed that 70% of the steam cracking plants combust hydrogen for thermal energy recovery purposes while 30% include the hydrogen in their product basket. When the co-produced hydrogen is combusted on-site, the corresponding amount of NG is displaced using the displacement method. For the share of hydrogen co-product that is included in the steam crackers' product basket, the emissions burdens associated with the steam cracking process is allocated to the hydrogen based on the mass share of hydrogen in the product basket.[1,17] This is consistent with the default setting implemented in the current version of the GREET model.[1,14] For the hydrogen combustion scenario, we assumed that the corresponding amount of NG is displaced due to the thermal energy recovered from the combustion of hydrogen. For those plants that include hydrogen in their product basket, we applied mass allocation method to hydrogen: we allocated the GHG emissions burdens associated with steam cracking to hydrogen based on the mass share of hydrogen in the product basket.[1,14] For the co-products other than hydrogen, mass allocation method is applied.[1,14]

Second, for the propylene sourcing mix, due to the lack of LCI dedicated to the PDH pathway, the CI of propylene produced from the FCC pathway is used as a proxy to represent the PDH pathway.[1,14] This is consistent with the default setting implemented in the current version of the GREET model.[1]

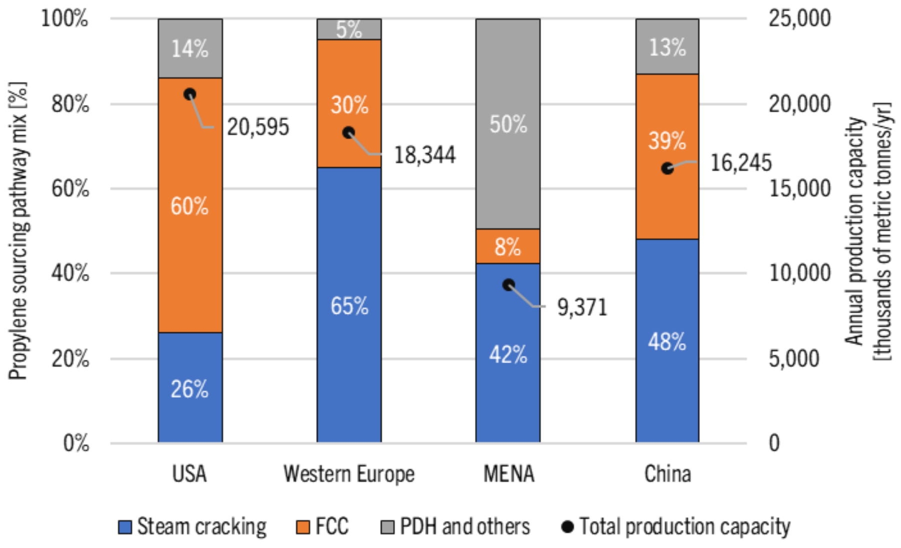

Figure 11. Shares of steam cracking, FCC, and PDH/other propylene sourcing pathway mix for each region with annual propylene production capacity.

2.5.3. Polyvinyl chloride (PVC)

For PVC, the following factors are identified to potentially vary its CI across the regions:

- CI of electricity in the region of PVC production;
- CI of NG production in the region of PVC production; and
- Technology share for VCM production.

Figure 12 shows the technology share for the VCM production in 2010 for each of the regions investigated in this study. All regions except for China used the VCM produced via EDC pathway while the VCM was dominantly produced via acetylene-pathway in China. The prevalence of acetylene-pathway for VCM production in China was attributed to the relative abundance of coal to derive the calcium carbide (CaC_2), which can then be converted to acetylene through the reaction with water.[12]

For PVC, the current version of GREET only contained the EDC-based PVC production.[1,21] Thus, the CI of PVC via acetylene pathway is estimated by addressing the differences in electricity and thermal energy consumption between the two (acetylene vs. EDC) pathways. Using a previously published work, the acetylene-based VCM pathway is assumed to consume 1.32 times the electricity and 1.95 times thermal energy compared to the EDC-based VCM pathway.[20]

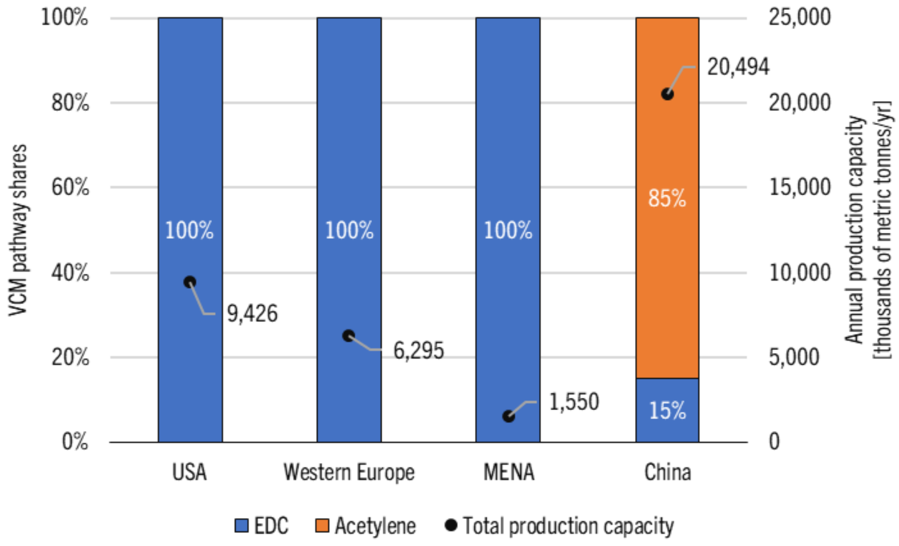

Figure 12. Shares of EDC- and acetylene-based VCM pathways for the PVC production in each region with annual PVC production capacity.

2.6. Data sources and assumptions for sensitivity analyses

2.6.1. Sensitivity analysis to address the timelines of the baseline datasets

For our baseline analysis, the CEH marketing research reports in the timeframe of 2010 to 2012 are referenced to collect the datasets regarding

- Terephthalic monomer pathway share in each region[8];
- Steam cracking feedstock mix in each region[30];
- Propylene sourcing technology mix in each region[31]; and
- VCM production technology mix in each region.[12]

To address the potential variation between the timeframe between 2010 and 2012 to a more recent timeframe (2019-2022), other publicly available resources were used to collect the datasets representing more recent years.

First, to estimate the progression of decreasing DMT share used in global PET production, the global DMT production in 2022 is referenced from a market report.[32] The DMT production in 2022 is compared to the DMT production in the CEH marketing research report published in 2010.[33] As a result of the comparison, the DMT production decreased by 56% between the two years. Thus, we applied the 56% reduction universally to all four regions to estimate the current DMT pathway share.

Second, to compare the steam cracking feedstock mix and propylene sourcing technology mix in 2010-2012 with those in 2019-2022 timeframe, Lopez et al.[34] is referenced for the 2019 timeframe. Gracida-Alvarez et al.[35] is referenced for the 2022 timeframe (only for the steam cracking feedstock mix in the USA). Although these datasets could supplement the datasets used for our baseline analysis (2010-2012 timeframe) by providing a more recent temporal context, it was difficult to replace the original baseline datasets because none of these studies provided datasets with identical regional definitions to our purposes. For example, Lopez et al.[34] provided the steam cracking feedstock mix and propylene sourcing technology mix for North America (i.e., USA, Canada, and Mexico), not for only the USA. They also did not provide the datasets dedicated to "Western" Europe and China, instead, their datasets were representing Europe as a whole and Northeastern Asia including China, Japan, Taiwan, and South Korea. Due to these differences in the definitions of regions, we decided to keep the datasets used for our baseline analysis and supplement the potential variation over time by conducting sensitivity analyses using the more recent supplementary datasets.

Figure 13 shows the terephthalic monomer shares for PET in each region assumed for our baseline analysis (2011) and more recent datasets (2022). The 56% reduction in DMT share is assumed for all four regions.[32,33] For China, the DMT share in PET production was already 0% in 2011 and, thus, remained at 0% for 2022.

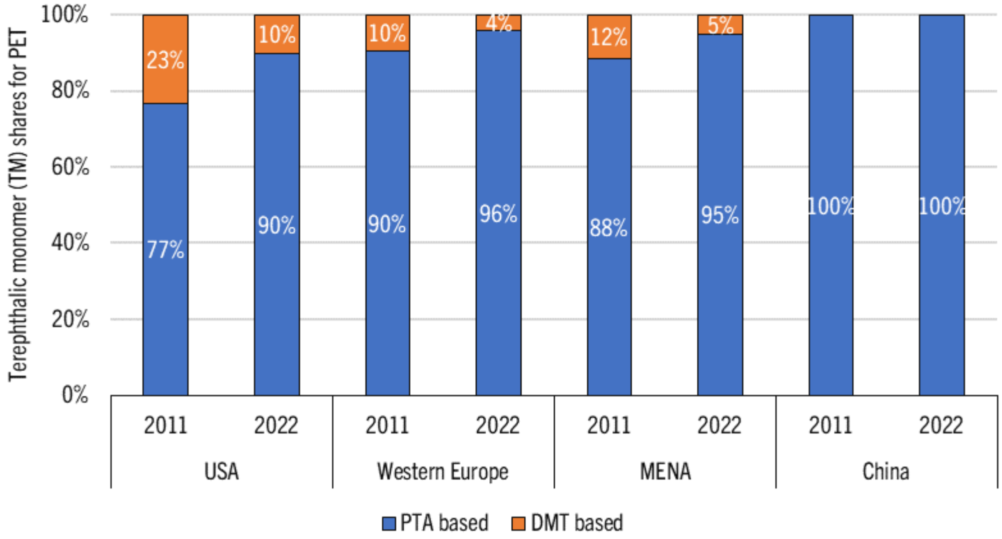

Figure 13. Estimated shares of PTA- and DMT-path for PET production in each region.

Figure 14 shows the steam cracking feedstock mix for each region assumed for our baseline analysis (2010) and more recent datasets (2019-2022 timeframe). For the USA, two different datasets are used to vary the share of NGL in the steam cracking feedstock mix from the baseline assumption. In all regions, there were no changes in the type of feedstock that took the majority of the steam crackers between 2010 and 2019-2022 timeframes. While NGL accounted for the majority of steam cracking feedstock in the USA and MENA for both baseline and sensitivity analyses, petroleum accounted for the majority of steam cracking feedstock in Western Europe and China for both baseline and sensitivity analyses.

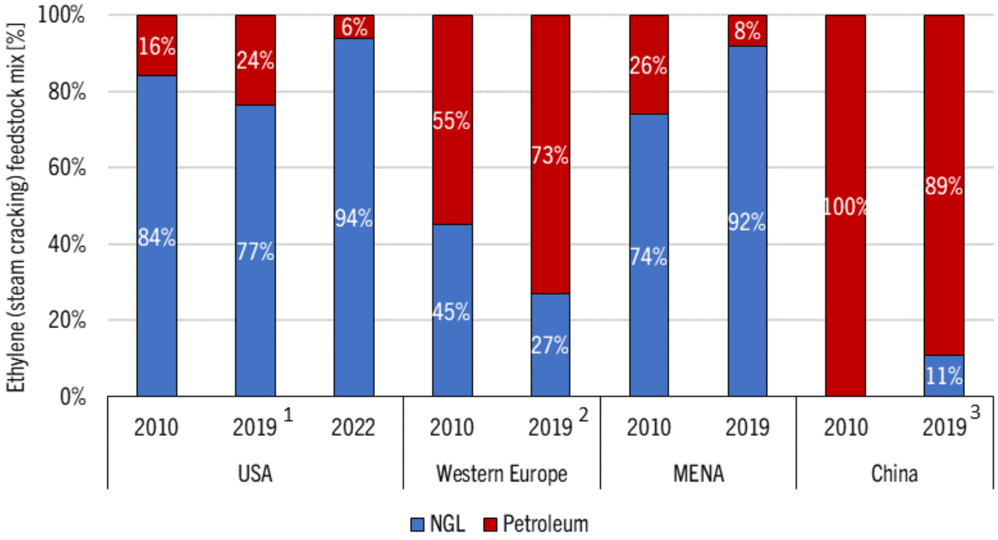

Figure 14. Estimated shares of NGL and petroleum-based products in the steam cracking feedstock mix in each region in 2019-2022 timeframe compared to the 2010 dataset (baseline). *There are some differences in the regions defined by the datasets used for sensitivity analysis: [1] North America; [2] Europe; [3] Northeastern Asia.

Figure 15 shows the propylene sourcing technology mix in each region assumed for our baseline analysis (2011) and more recent dataset (2019). For all regions, the technology that accounted for the majority of propylene production in 2011 still accounted for the majority of propylene in 2019. In the USA and MENA, non-steam cracking pathways such as FCC and PDH accounted for the majority of propylene in both 2011 and 2019, while, in Western Europe, steam cracking was the prevalent technology to produce propylene in both 2011 and 2019. In China, steam cracking and non-steam cracking pathways accounted for about half of the propylene production, respectively in both 2011 and 2019.

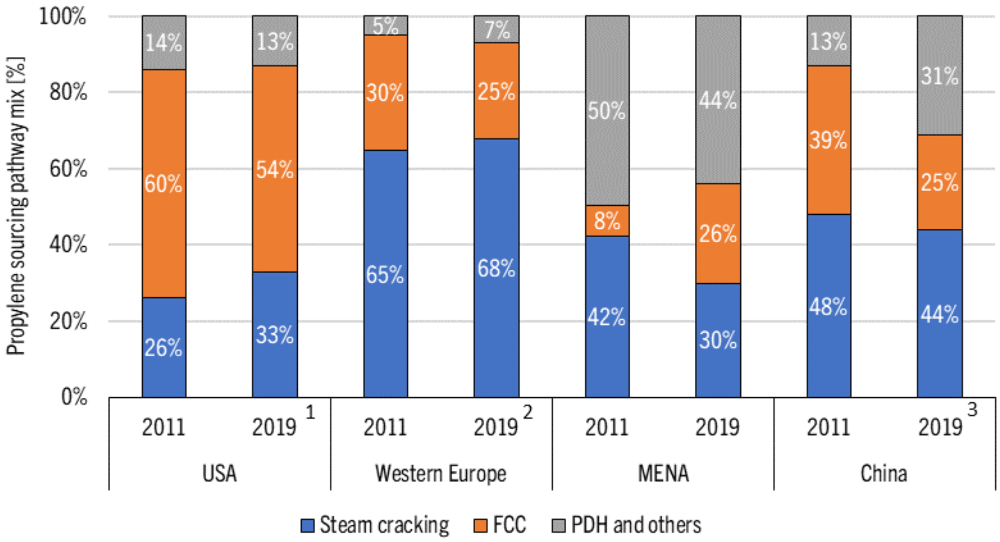

Figure 15. Estimated shares of steam cracking, FCC, and PDH/other propylene sourcing pathway mix for each region in 2019 timeframe compared to the 2011 dataset (baseline). Other propylene sourcing pathways include ethylene/butylene metathesis, coal-based Fischer-Tropsch and vacuum gas oil processing.[1] North America; [2] Europe; [3] Northeastern Asia.

For PVC, we validated that the following two facts are still relevant for the recent years based on reliable resources[36,37]: i) China is the only region that uses acetylene-based VCM production technology in all four regions of interest in this study; and ii) acetylene-based VCM production technology is a dominant path to produce VCM in China. Thus, we did not conduct sensitivity analysis on the variation in the acetylene pathway share in VCM production.

2.6.2. Sensitivity analysis to address the hydrogen use scenario in steam cracking process

As mentioned before, the baseline analysis assumed the share of hydrogen combustion in steam crackers as 70%: 70% of the steam crackers in all regions combust its co-produced hydrogen for thermal energy recovery while the rest do not.[1,14] However, this share can vary across the regions. In this study, to estimate the potential impacts of regional variation in the hydrogen use-scenario, a sensitivity analysis is conducted by varying the share of combusted hydrogen between 0% and 100%. The results are presented in Section 3.2.4.

3. Results and Discussion

3.1 Cradle-to-gate GHG emissions results

3.1.1. Polyethylene terephthalate (PET)

Figure 16-(a) shows the cradle-to-gate GHG emissions results for PET production in four regions. The figure shows the contributions from different processes based on the color code: i) the polymerization process (red); ii) the EG production (blue); and iii) the terephthalic monomer production (yellow). The impact of each process is further broken down into the contribution of each of the processes' input material and energy. The contributions from each of the material and energy inputs can be noted by different fill patterns: i) solid fill for the contributions from electricity inputs; ii) diagonal stripe pattern fill for the contributions from NG inputs; and iii) checker pattern fill for the contributions from materials inputs. For the readers interested in the impacts categorized by electricity, NG, and materials, please refer to Figure 17 where the legend categories with the same fill patterns are grouped together. In Figure 16-(a), the average of the PET's CI across the four regions is also presented (in dashed line), and the deviation from this cross-regional average for each of the four regions is shown in Figure 16-(b). The same color code and fill patterns are used in Figure 16-(b) as Figure 16-(a) to show the contributions from each legend to the total deviation.

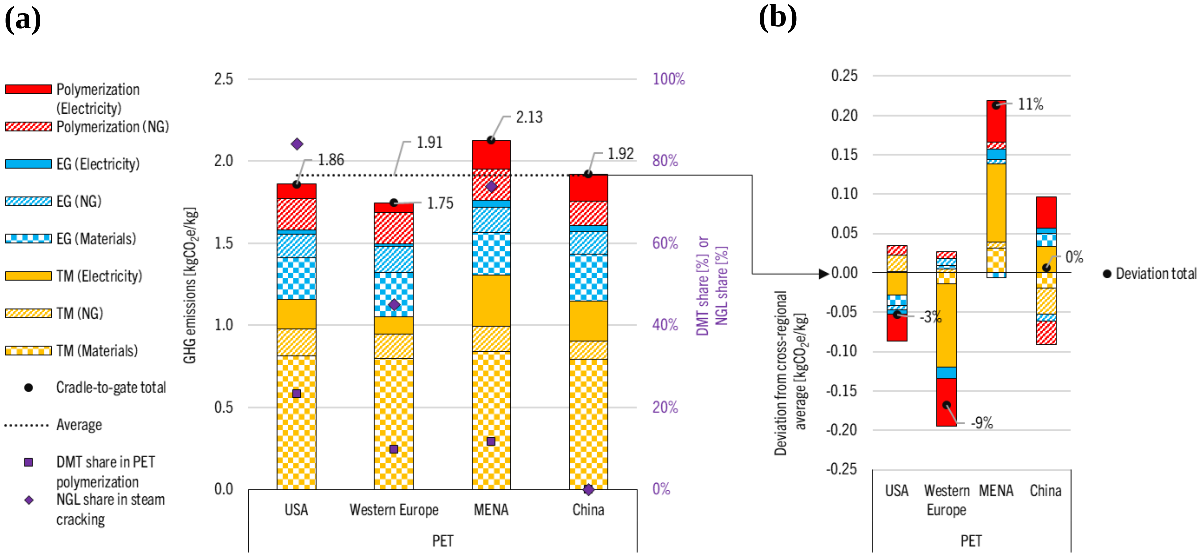

Figure 16. (a) Cradle-to-gate GHG emissions results for PET in four regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average.

In Figure 16-(a), we can see that the CI of PET increases in the order of "Western Europe < USA < China < MENA". There was a moderate degree of variation across the four regions (up to 11% higher in MENA and up to 9% lower in Western Europe relative to the cross-regional average). Figure 16-(b) shows the origins of this cross-regional differences in PET's CI.

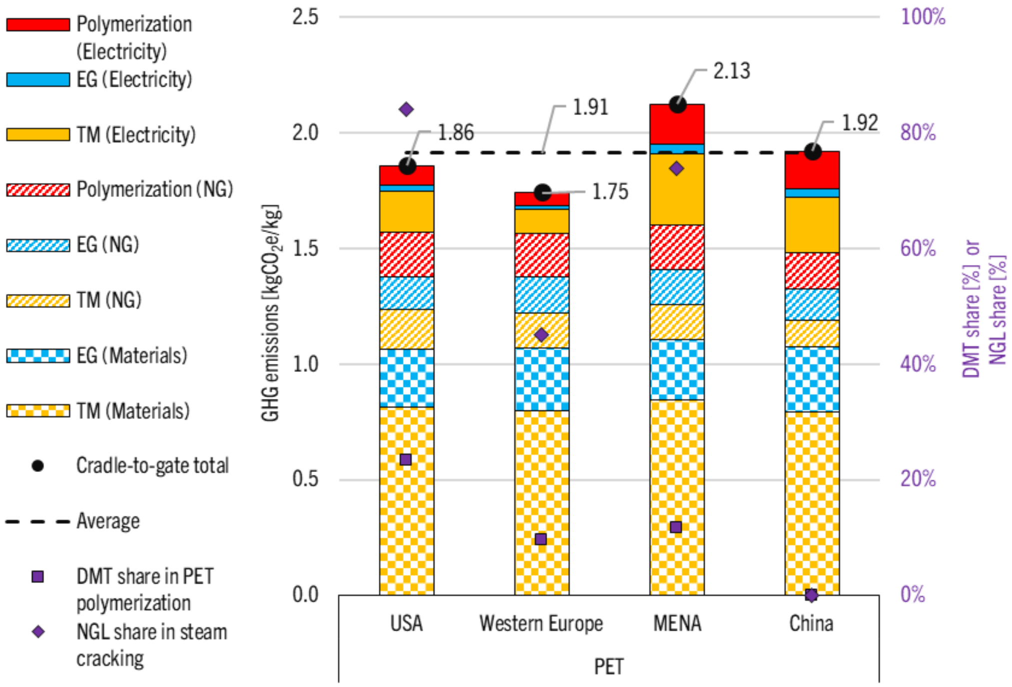

Figure 17. Cradle-to-gate GHG emissions results for PET in four different regions (breakdown categories organized by the same fill patterns).

The variations in PET's CI across the four regions were mainly due to the regional differences in the GHG emissions from electricity usage (solid fill), which was mainly due to the regional variation in CI of electricity. The CI of electricity across the four regions is presented in Figure 18-(a). Here, we can see that the trend of CI of electricity across the four regions ("Western Europe < USA < China < MENA") is consistent with the trend of PET's cradle-to-gate CI shown in Figure 17. In this study, we have also investigated how the different CI of NG production in each region [see Figure 18-(b)] affects the PET's CI across the four regions. However, this impact was relatively smaller than the impact caused by the regional electricity CI variation.

Although the majority of cradle-to-gate GHG emissions from PET production is from the impacts of material inputs (see Checker fill patterns in Figure 17) in different processes [i.e., "EG (materials)" and "terephthalic monomer (materials)"], the GHG emissions associated with these material inputs did not have significant differences across the four regions.

The other two possible variations across the four regions of PET production considered in this study are the differences in i) DMT-path share in each region's PET mix; and ii) steam cracking feedstock mix (NGL vs. petroleum). Each region's DMT-path share (purple square) and NGL share in steam cracking feedstock (purple diamond) is shown in Figure 17. Although we took these two factors into account in this study, the impacts of these two factors were not as dominant as those from the CI of electricity. Since the DMT-based PET production (2.39 $kgCO_2e/kg$-PET) is more carbon-intensive than the PTA-based PET production (1.92 $kgCO_2e/kg$-PET), those regions with higher DMT-path share were expected to result in higher CI of PET than the regions with lower DMT-path share if all other conditions are constant. However, all investigated regions' DMT-path share was low, thus its impact being overshadowed by more important factors such as the CI of electricity. For example, the USA has the highest DMT-path share (23%) across the four regions. However, the CI of PET produced in USA was lower than MENA and China because the impact of DMT-path is overshadowed by the USA's lower CI of electricity relative to those two regions.

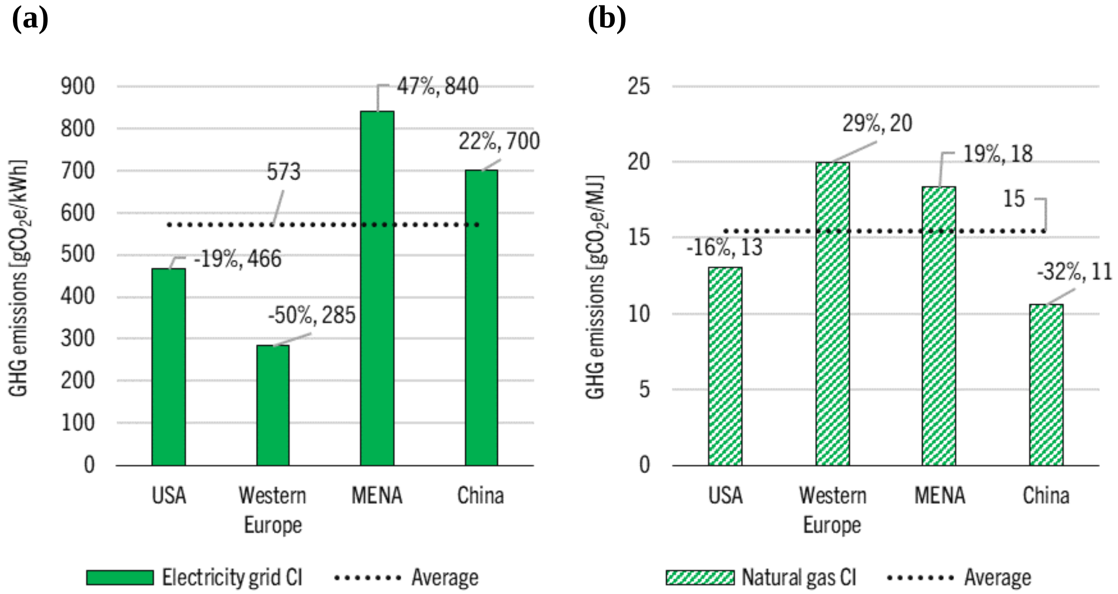

Figure 18. Carbon intensity of (a) electricity grid in four regions; and (b) NG production in four regions. The numbers in % means the deviation from the cross-regional average.

The type of feedstocks used for steam cracking was also not the trend-setter for the PET's CI across the four regions. As shown in Figure 19, the CI of ethylene is lower when it is produced from NGL feedstock (1.03 $kgCO_2e$/kg-ethylene) than from petroleum feedstock (1.19 $kgCO_2e$/kg-ethylene). Thus, the regions with higher NGL share in its steam cracking feedstock were expected to result in lower CI for ethylene resulting in lower CI for EG and then PET when all other conditions are constant. However, due to the more important factors such as the CI of electricity, the impact of steam cracking feedstock is overshadowed. For example, MENA has a much higher NGL share in its steam cracking feedstock mix compared to the Western Europe. However, the GHG emissions benefits of using NGL over petroleum in steam cracking are overshadowed by their carbon-intensive electricity grid compared to Western Europe, thus resulting in 22% higher cradle-to-gate GHG from PET production compared to Western Europe.

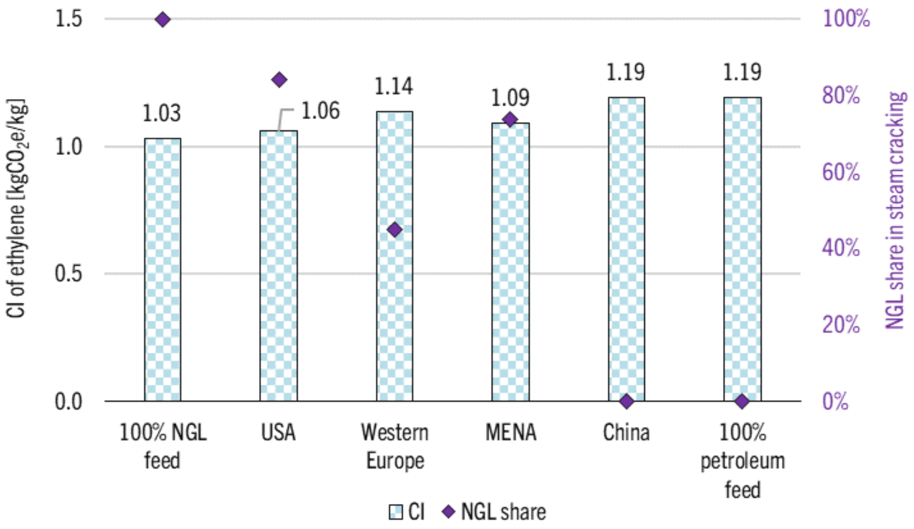

Figure 19. Carbon intensity of ethylene produced in four different regions. CI of ethylene production solely from either NGL or petroleum feedstock is presented for comparison purposes. Note: for the 100% NGL and petroleum feed cases, USA electricity grid mix and NG production are assumed.

3.1.2. High-Density Polyethylene (HDPE)

Figure 20-(a) shows the cradle-to-gate GHG emissions from HDPE production in the four regions. Different processes (i.e., polymerization and olefin monomer production) are marked with different colors while different material and energy inputs are noted with different pattern fills. The average across the four regions are also presented with a black dashed line. The NGL share in each region's steam cracking feedstock mix is presented with purple diamond. The CI of HDPE increases in the order of USA < Western Europe < MENA < China. There was a moderate degree of variation across the four regions [see Figure 20-(b)]: 7% higher in China and 7% lower in USA relative to the cross-regional average. Figure 20-(b) also shows the origins of this cross-regional difference in HDPE's CI.

The HDPE's cross-regional difference in CI could be attributed to two main reasons: the differences in the i) electricity-associated GHG emissions; and ii) CI of ethylene. Since it is assumed that all four regions have identical electricity consumption during the polymerization process for HDPE production, the difference in electricity relevant GHG emissions is solely from the regional difference in the CI of electricity. The region with the highest NGL share in its steam cracking feedstock mix (i.e., USA) had the lowest CI of ethylene while the region with the lowest NGL share (i.e., China) had the highest CI of ethylene (see Figure 19). This is combined with the CI of electricity and resulted in the rank order of CI of HDPE across the four regions.

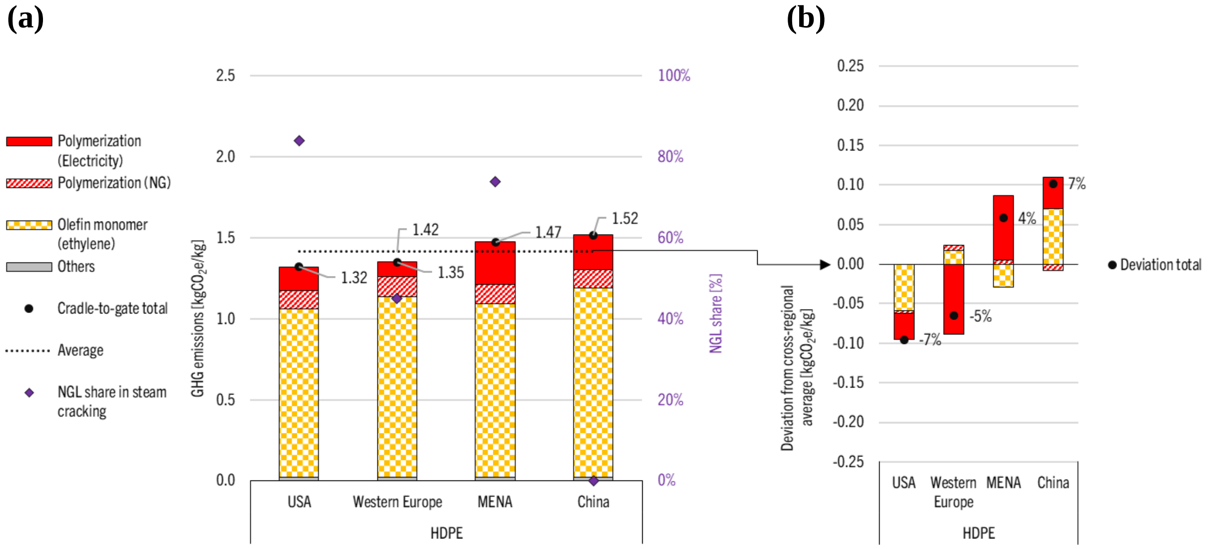

Figure 20. (a) Cradle-to-gate GHG emissions results for HDPE in four different regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average. The "Others" legend category includes all other material inputs (e.g., nitrogen gas, silica gel, etc.) required for HDPE polymerization than olefin monomer.

3.1.3. Low-Density Polyethylene (LDPE)

Figure 21-(a) shows the cradle-to-gate GHG emissions from the LDPE production in the four regions. Different processes (i.e., polymerization and olefin monomer production) are marked with different colors while different material and energy inputs can be noted with different pattern fills. The average across the four regions are also presented with black dashed line. The NGL share in each region's steam cracking feedstock mix is presented with purple diamond. The CI of LDPE increases in the order of Western Europe < USA < China < MENA. There was a moderate degree of variation across the four regions [see Figure 21-(b)]: 9% higher in MENA and 9% lower in Western Europe relative to the cross-regional average. Figure 21-(b) also shows the origins of this cross-regional difference in LDPE's CI.

Most of the LDPE's cross-regional difference in CI could be attributed to two main reasons: the differences in the i) electricity-associated GHG emissions; and ii) CI of ethylene. Since it is assumed that all four regions have identical electricity consumption during the polymerization process for LDPE production, the difference in electricity relevant GHG emissions is solely from the regional difference in the CI of electricity. The region with the highest NGL share in its steam cracking feedstock mix (i.e., USA) had the lowest CI of ethylene while the region with the lowest NGL share (i.e., China) had the highest CI of ethylene (see Figure 19). This is combined with the CI of electricity and resulted in the rank order of CI of LDPE across the four regions. Compared to the HDPE results, for LDPE, the impact of regional CI of electricity was noticeably higher than that of regional CI of ethylene because of the higher electricity consumption required for LDPE production relative to HDPE.

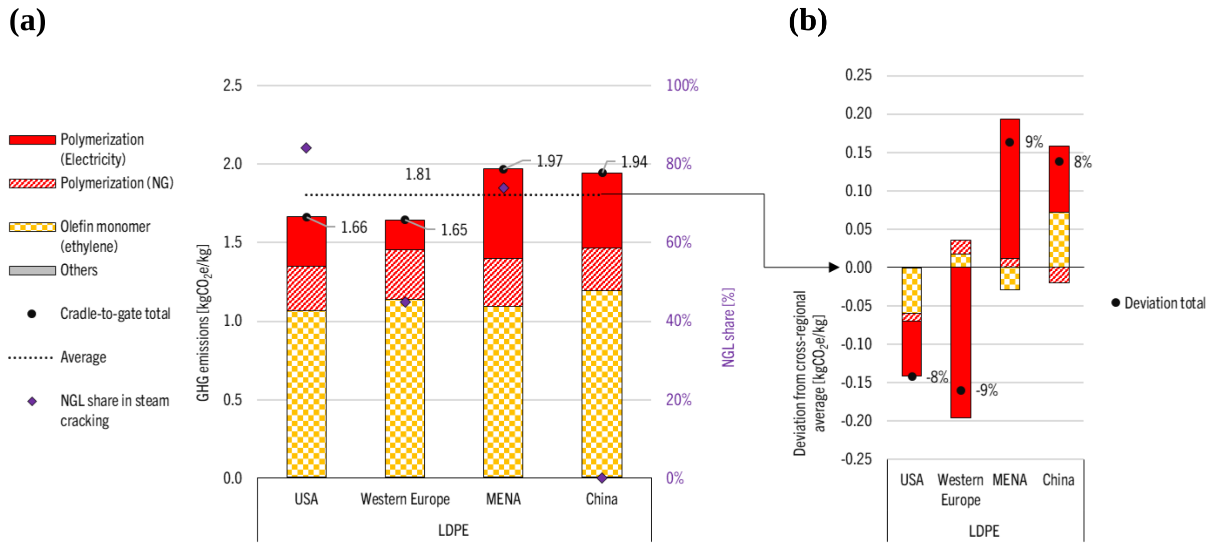

Figure 21. (a) Cradle-to-gate GHG emissions results for LDPE in four different regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average. The "Others" legend category includes all other material inputs (e.g., nitrogen gas) required for LDPE polymerization than olefin monomer.

3.1.4. Polypropylene (PP)

Figure 22-(a) shows the cradle-to-gate GHG emissions from the PP production in the four regions. Different processes (i.e., polymerization and olefin monomer production) are marked with different colors while different material and energy inputs can be noted with different pattern fills. The average across the four regions are also presented with black dashed line. The NGL share in each region's steam cracking feedstock mix is presented with purple diamond, and the share of propylene sourced from steam cracking is presented with purple square. The other pathways than steam cracking to source propylene are FCC and PDH.

The CI of PP increases in the order of USA < Western Europe ≈ MENA < China. There was a moderate degree of variation across the four regions [see Figure 22-(b)]: by 3% higher in China and by 8% lower in the USA relative to the cross-regional average. Figure 22-(b) also shows the origins of this cross-regional difference in PP's CI.

Most of the cross-regional differences in PP's CI could be attributed to two main reasons: the differences in the i) electricity-associated GHG emissions; and ii) CI of propylene. Since it is assumed that all four regions have identical electricity consumption during the polymerization process for PP production, the difference in electricity relevant GHG emissions is solely from the regional difference in the CI of electricity. Since the CI of propylene produced from non-steam cracking processes such as FCC or PDH is lower than that from steam cracking process (see Figure 23), the regions with lower steam cracking share in propylene sourcing had lower CI for their propylene which was one of the greatest factors that affected the CI of PP. The other important factor that affected the CI of PP was the regional CI of electricity. The regions with lower CI of electricity resulted in lower GHG emissions from its electricity usage. These two factors combined (i.e., CI of electricity and propylene) resulted in the current rank order shown for the CI of PP across the four regions. Compared to the HDPE and LDPE results, PP results were more dependent on the CI of olefin (propylene) than on the CI of electricity due to the lower electricity consumption required during the PP polymerization compared to HDPE or LDPE polymerization.

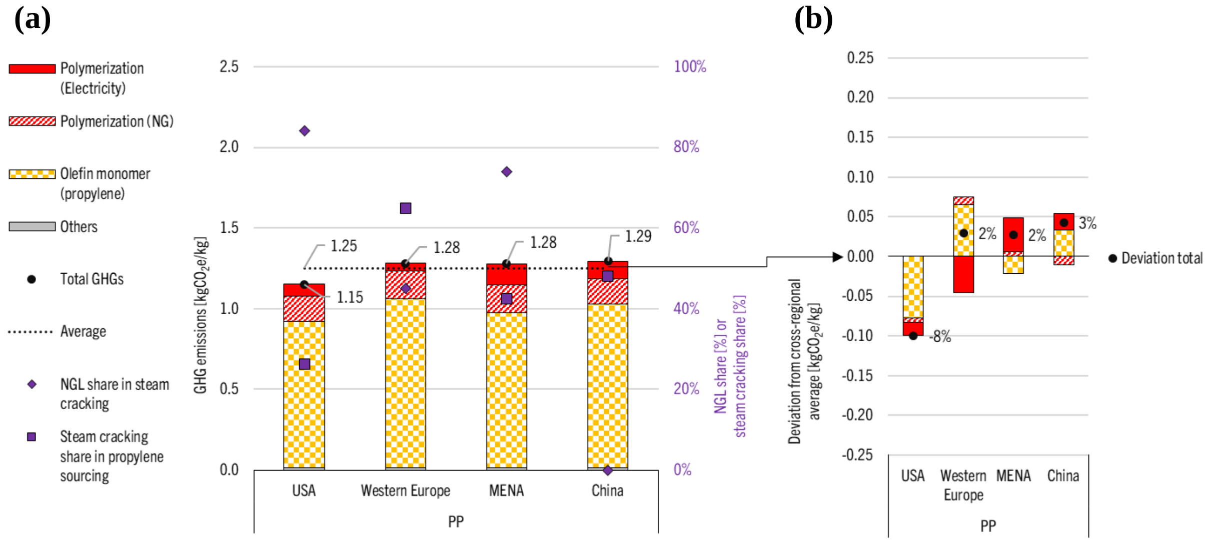

Figure 22. (a) Cradle-to-gate GHG emissions results for PP in four different regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average. The "Others" legend category includes all other material inputs (e.g., nitrogen gas) required for PP polymerization than olefin monomer.

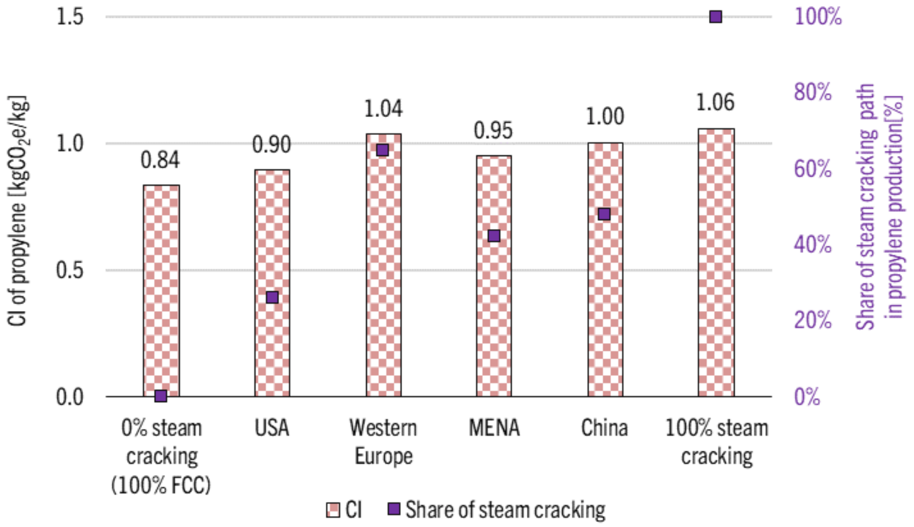

Figure 23. Carbon intensity of propylene produced in four different regions. CI of propylene production solely from either fluid catalytic cracking (FCC) or from steam cracking is presented for comparison purposes. Note: for the 0% and 100% steam cracking cases, USA electricity grid mix and NG production are assumed.

3.1.5. Polyvinyl chloride (PVC)

Figure 24-(a) shows the cradle-to-gate GHG emissions from PVC production in the four regions. Due to the different data structures of the LCI used for the LCA of PVC, the results are shown differently from the other four resins presented in the previous sections. For PVC, each material and energy input used for the entire cradle-to-gate cycle is separately labeled in each legend category with different color code in Figure 24. This is because the current version of the GREET model does not account for the inputs required for PVC production on a process level; it only addresses the inputs for the cradle-to-gate cycle. The average across the four regions are also presented with black dashed line. The acetylene-path share in each region's PVC production is presented with a purple square.

The CI of PVC increases in the order of Western Europe < USA < MENA < China. Unlike the other four resins that only showed a moderate degree of variation in its CI across the four regions, PVC showed a significant regional variation in its CI [see Figure 24-(b)]: up to 34% higher in China and up to 17% lower in Western Europe relative to the cross-regional average. Figure 24-(b) also shows the origins of this cross-regional difference in PVC's CI.

Most of this cross-regional difference could be attributed to two main reasons: the differences in the i) electricity-associated GHG emissions; and ii) NG-associated GHG emissions. For both electricity- and NG-associated GHG emissions during the PVC production, the acetylene-path share was a significant determinant affecting both the electric and thermal energy consumption. Compared to the EDC-path, the acetylene-path consumed 32% more electricity and 95% more NG.[20] The increase in electricity and thermal energy consumption during the PVC production combined with the higher CI of electricity in China have resulted in a significantly higher CI of PVC in China than the cross-regional average.

Figure 25 compares the CI of PVC produced via 100% acetylene-pathway or via 100% EDC-pathway in each of the two regions (i.e., USA and China) using each of the regions' electricity grid mix and NG production CI. As we can see from this figure, the simulated CI of PVC produced in China via 100% EDC pathway is only about 7% higher than its USA counterpart despite the differences in the CI of electricity and NG production. However, when the actual EDC path share (15%) in China is applied, the CI of PVC in China is significantly increased, which clearly shows the environmental impact of choosing acetylene pathway over the EDC pathway. The high CI of acetylene-based PVC production is mainly because the acetylene is sourced from the calcium carbide (CaC_2) which, in turn, is sourced from coal.[12]

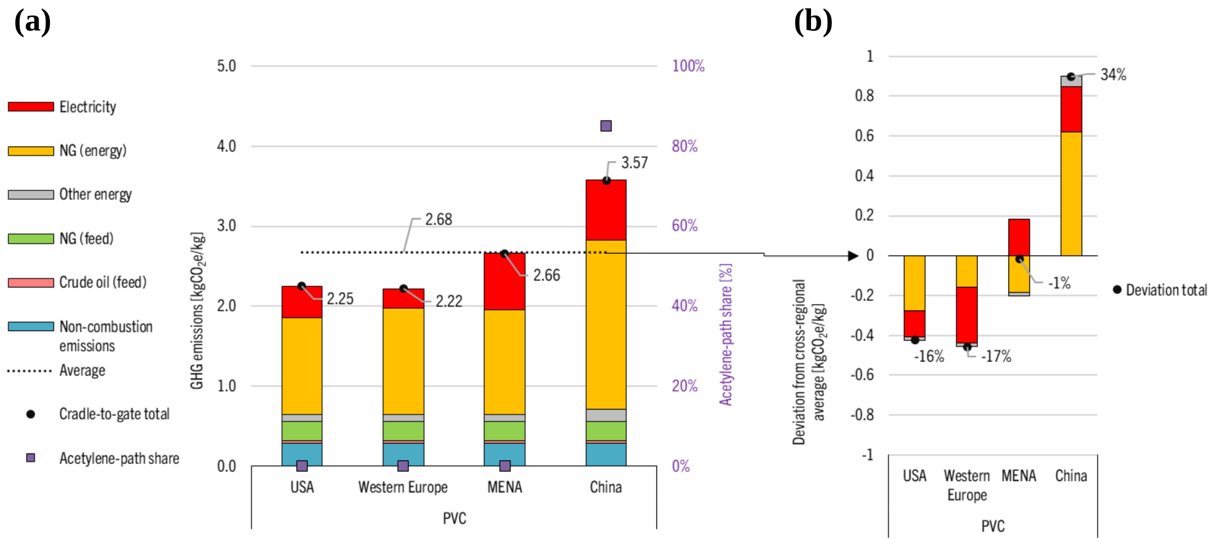

Figure 24. (a) Cradle-to-gate GHG emissions results for PVC in four different regions; (b) Each region's deviation in cradle-to-gate GHG emissions results from the cross-regional average

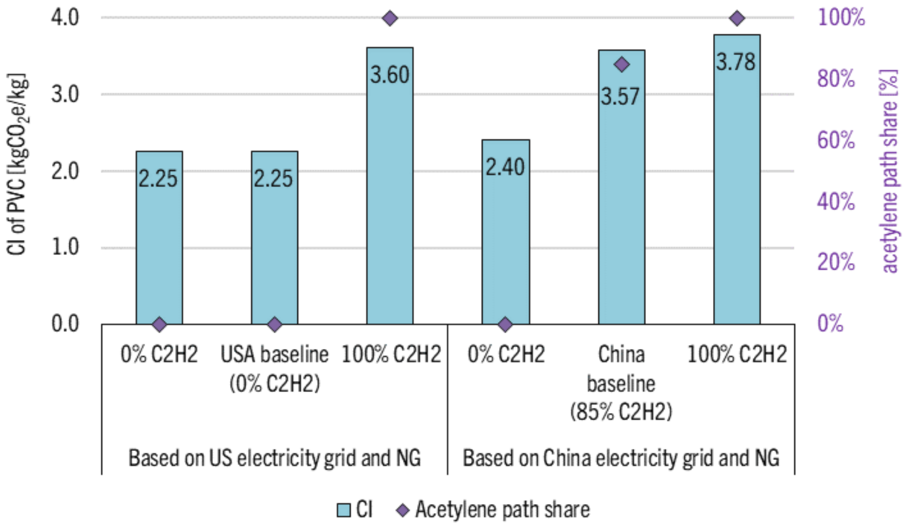

Figure 25. Carbon intensity of PVC produced in US and China compared to the CI of PVC produced solely from either acetylene-path or ethylene-path in each region.

3.1.6. CI of regionalized resin and olefin production pathways

Table 5 summarizes the list of dedicated pathways depending on different user-choices available in the GREET model[1] and the CI of the products produced from each of those pathways. For example, the “PTA-based PET CI” means the CI of PET produced solely based on the PTA technology pathway. When produced using the USA electricity generation mix and NG production, the CI of PET through the PTA pathway is 1.92 kgCO$_2$e/kg-PET.

Table 5: Summary of the CI for separate technology and feedstock.

Products	Technologies and feedstocks variations	Geography for electricity grid mix and NG production settings	Pathways	Carbon Intensity	Units
PET	Terephthalic monomer mix	USA	PTA-based	1.75	[kgCO$_2$e/kg-PET]
			DMT-based	2.23	
		Western Europe	PTA-based	1.70	
			DMT-based	2.22	
		MENA	PTA-based	2.07	
			DMT-based	2.58	
		China	PTA-based	1.92	
			DMT-based	2.39	
Ethylene and propylene	Steam cracking feedstock mix	USA	NGL-based	1.03	[kgCO$_2$e/kg-ethylene or propylene]
			Petroleum-based	1.19	
		Western Europe	NGL-based	1.05	
			Petroleum-based	1.19	
		MENA	NGL-based	1.05	
			Petroleum-based	1.19	
		China	NGL-based	1.02	
			Petroleum-based	1.19	
Propylene	Propylene sourcing mix	USA	Steam cracking-based	1.06	[kgCO$_2$e/kg-propylene]
			Non-steam cracking based (e.g., FCC and PDH)	0.84	
		Western Europe	Steam cracking-based	1.14	
			Non-steam cracking based (e.g., FCC and PDH)	0.85	
		MENA	Steam cracking-based	1.09	
			Non-steam cracking based (e.g., FCC and PDH)	0.85	
		China	Steam cracking-based	1.19	
			Non-steam cracking based (e.g., FCC and PDH)	0.83	
PVC	VCM production technology mix	USA	EDC-based	2.25	[kgCO$_2$e/kg-PVC]
			Acetylene-based	3.60	
		Western Europe	EDC-based	2.22	
			Acetylene-based	3.64	
		MENA	EDC-based	2.66	
			Acetylene-based	4.20	
		China	EDC-based	2.40	
			Acetylene-based	3.78	

3.2. Sensitivity Analysis

3.2.1. Impact of potential variation in the DMT-path share

Figure 26 shows the PET's cradle-to-gate CI assuming different DMT-path shares from what is assumed for our baseline results. For our baseline results, we assumed that the DMT-path shares in each region will be 23%, 10%, 12%, and 0% for USA, Western Europe, MENA, and China, respectively. To account for the fact that this DMT-path share is based on the 2011 dataset, we applied a different set of DMT-path share to each region to represent the 2022 context: 10%, 4%, 5%, and 0% for USA, Western Europe, MENA, and China, respectively. Then, we compared the resulting CI of PET to our baseline results.

As we can see from Figure 26, the impact of varying the DMT-path share of PET to a more recent year estimation was minimal in all four regions. The USA was the region where the impact was the greatest, which is only a 3% decrease from the baseline value. This small impact of adjusting the DMT-path share to a more recent estimation seems to be due to an already small share of DMT-pathway in year 2011, which did not leave much room for improvement in PET's CI by reducing DMT-path share.

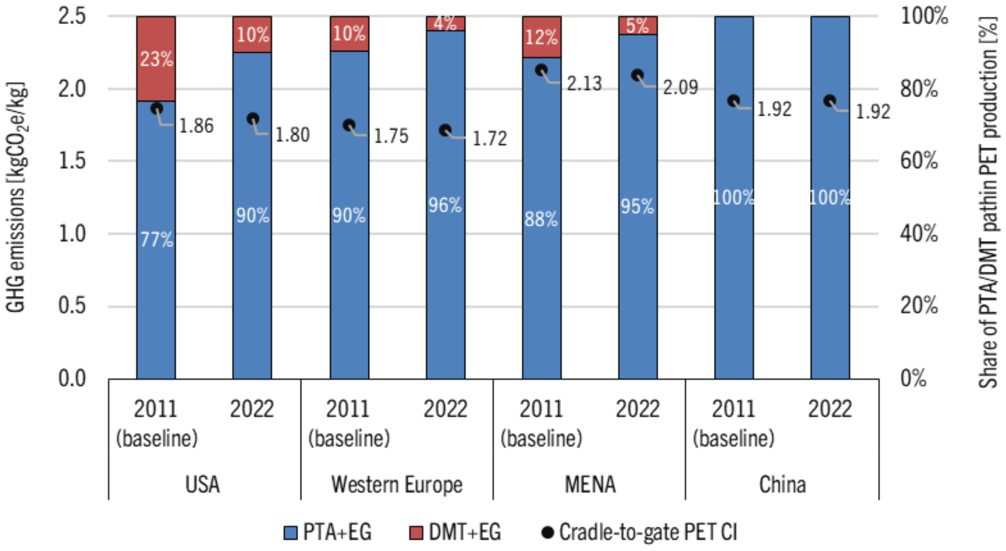

Figure 26. Sensitivity analysis results on PET CI using the 2022 estimation on the DMT-path share in PET production.

3.2.2. Impact of potential variation in the steam cracking feedstock mix

Figure 27 shows the cradle-to-gate CI of HDPE and LDPE using more recent datasets for the steam cracking feedstock mix. As we can see from Figure 27, the impact of varying the steam cracking feedstock mix to represent 2019 or 2022 timeframe was minimal. In all regions, the degree of impact on the CI of HDPE or LDPE was less than 2%. Although many regions experienced a noticeable change in the NGL share in each of their steam cracking feedstock mix, that impact was not noticeable from a cradle-to-gate CI perspective.

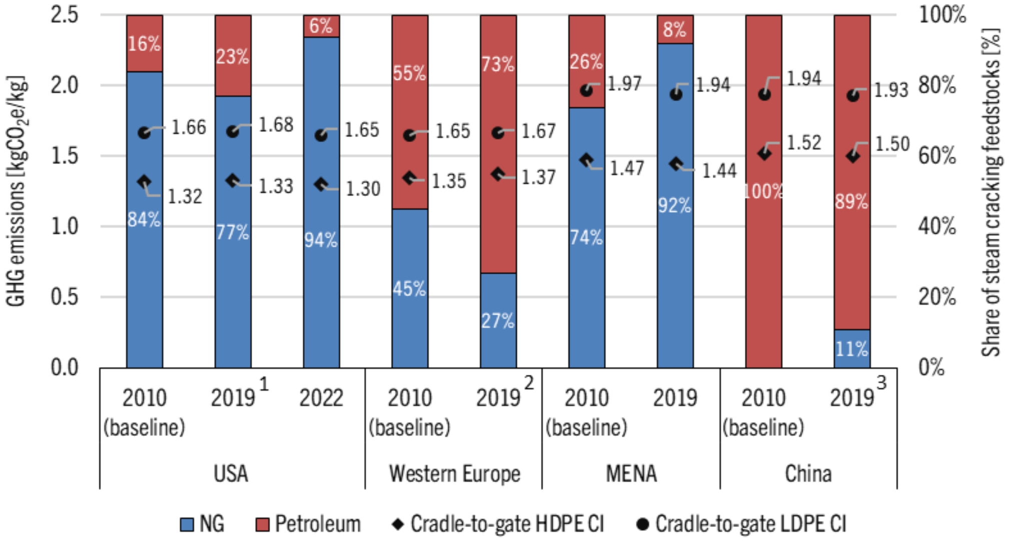

Figure 27. Sensitivity analysis results on HDPE and LDPE CIs using the 2019-2022 estimation on the NGL-share in steam cracking feedstock. *There are some differences in the regions defined by the datasets used for sensitivity analysis: ^{1} North America; ^{2} Europe; ^{3} Northeastern Asia.

3.2.3. Impact of potential variation in propylene sourcing mix

Figure 28 shows the cradle-to-gate CI of PP with a different propylene sourcing mix to represent a more recent timeframe (2019) than what is assumed for our baseline results. Although there are some variations in how much share of propylene is sourced from steam cracking between the baseline assumption and the assumption representing 2019 timeframe, there is no significant change in the CI of PP between the two scenarios (less than 1.3% in all regions).

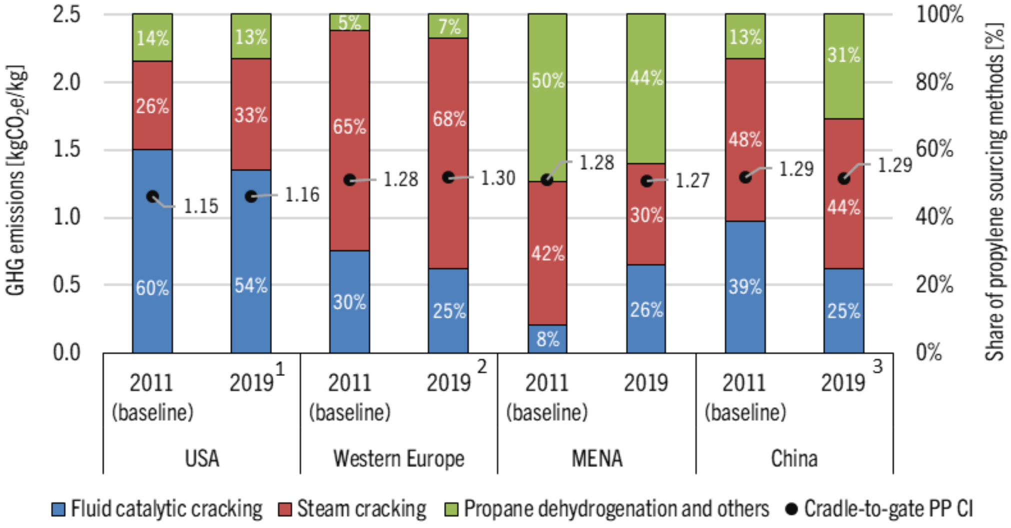

Figure 28. Sensitivity analysis results on PP CI using the 2019 estimation on the steam cracking path share in propylene production. *There are some differences in the regions defined by the datasets used for sensitivity analysis: [1] North America; [2] Europe; [3] Northeastern Asia.

3.2.4. Impact of variation in hydrogen use scenario in steam cracking plants.

Figure 29 shows the cradle-to-gate CI of (a) PET, (b) HDPE and LDPE, and (c) PP with different assumptions on the hydrogen use scenario during the steam cracking. To investigate the impact of the hydrogen use scenario in the steam cracking process, the CI of different resins are calculated assuming 0% and 100% hydrogen use for energy recovery in each region. The percentage variation from the baseline is shown as the data label in each bar.

The result shows that, for PET, the impact of varying hydrogen use scenario is minimal: less than 3% from a perspective of the cradle-to-gate CI of PET. However, for polyolefins such as HDPE, LDPE, and PP, the impact of varying hydrogen use scenario was significant. Thus, collecting datasets on the hydrogen use scenario in each different region would be important for better accuracy in the regionalized LCA results on these polyolefins.

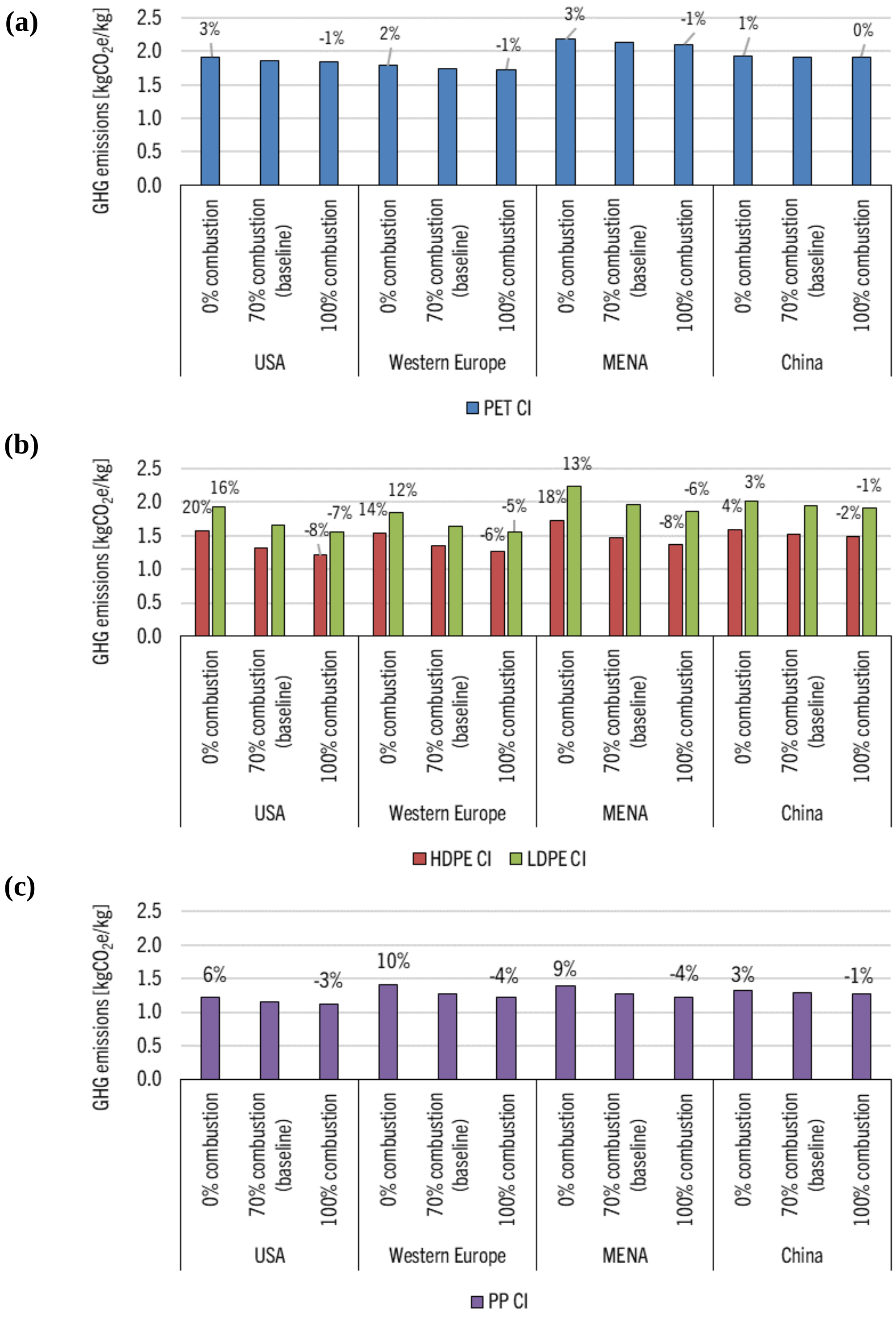

Figure 29. Sensitivity analysis results on PET, HDPE, LDPE, and PP CI by varying the hydrogen use scenario in the steam cracking of olefin.

4. Summary and Conclusions

In this study, the CIs of five different resins, PET, HDPE, LDPE, PP, and PVC, are investigated in four regions: USA, Western Europe, MENA, and China. The regional factors such as the CI of electricity and NG production, shares of terephthalic monomer type in PET production, steam cracking feedstock mix, propylene sourcing technology mix, and VCM production technology mix are identified to estimate the CI of resins for each of the four regions. The datasets for the above factors were collected from different marketing research reports, journal articles, and industry/governmental websites.

For each resin, its CI increased in the order shown in **Table 1**. The results showed that there is a moderate degree of variation in the CI of the PET, HDPE, LDPE, and PP across the four regions. However, the cross-regional variation for PVC was significant. Usually, resins produced in the USA or Western Europe exhibited lower CI than those produced in MENA or China due to the lower CI of electricity grid in USA or Western Europe.

Out of the factors affecting the regional variations in the CI of resins, the CI of electricity was one of the most impactful factors affecting the resin's cradle-to-gate CI. Although electricity was not the major contributor on the studied resins' GHG emissions on a cradle-to-gate basis, the degree of variation in the GHG emissions associated with electricity consumption was significant across different regions due to a significantly different regional CI of electricity.

In addition, for polyolefins, CI of the olefins was another important factor affecting the CI of resin in each region. For example, the CI of HDPE was significantly dependent on the CI of ethylene which, in turn, was affected by the steam cracking feedstock mix in each of the regions studied in this work. For those regions with higher NGL share in its steam cracking feedstock mix, the CI of ethylene was lower than those regions with higher petroleum share, thus resulting in relatively a lower CI of HDPE in that region. For PVC, the technological pathway used to produce its monomer (the VCM) was the important factor determining the region's CI of PVC. If the regional share for acetylene-based VCM production was higher, that led to the higher CI for PVC due to the higher electrical and thermal energy consumption associated with acetylene pathway compared to the EDC pathway.

In the current study, although many different variables that can potentially cause the regional variations in the CI of resins were investigated, the list of variables was not exhaustive. Through sensitivity analysis, the impact of different hydrogen use scenarios in each region was investigated. The results showed that whether the hydrogen in the tail gas from the steam cracking process is combusted to provide process heat or exported as a coproduct can cause significant variations in the CI of the polyolefins (i.e., HDPE, LDPE, PP). Thus, the use of the hydrogen co-product from the steam cracking process in each region would be important to characterize.

Through this research, we learned that the methods used for the current research could be replicated to produce additional regionalized plastic production pathways for other regions and resins. For future work, we suggest expanding the research to collect region-specific LCI for each technological pathway to address any regional or technological differences in energy and material consumptions for these pathways.

5. References

[1] GREET: Greenhouse Gases, Regulated Emissions, and Energy use in Technologies, 2022. Argonne National Laboratory. http://greet.es.anl.gov (accessed in November 2023).

[2] Cabernard, L.; Pfister, S.; Oberschelp, C.; Hellweb, S. Growing environmental footprint of plastics driven by coal combustion, *Nature Sustainability*, 2022, 5, 139-148. DOI: 10.1038/s41893-021-00807-2.

[3] Hermanns, R.; Meys, R.; Katelhon, A.; Stellner, L.; Vogler, O.; Bardow, A.; Suh, S. *New LCI Database for Chemicals and Plastics*; 2021 ACLCA Conference, September 2021.

[4] Organisation for Economic Co-operation and Development (OECD) website; *Plastic leakage and greenhouse gas emissions are increasing*; https://www.oecd.org/environment/plastics/increased-plastic-leakage-and-greenhouse-gas-emissions.htm#:~:text=In%202019%2C%20plastics%20generated%201.8,and%20conversion%20from%20fossil%20fuels. (Accessed on June 16th, 2023).

[5] Geyer, R.; Jambeck, J.R.; Law, K.L. Production, use, and fate of all plastics ever made, *Science Advances*, 2017, 3, 31700782. DOI: 10.1126/sciadv.1700782.

[6] Nicholson, S.R.; Rorrer, N.A.; Carpenter, A.C.; Beckham, G.T. Manufacturing Energy and Greenhouse Gas Emissions Associated with Plastics Consumption, *Joule*, 2021, 5, 673-686. DOI: 10.1016/j.joule.2020.12.027.

[7] *Chemical Upcycling of Polymers*; Report of the Basic Energy Sciences Roundtable; Department of Energy: Washington, D.C.; 2019.

[8] Sesto, B.; Kumamoto, T. *PET Polymer - Chemial Economics Handbook (CEH) Marketing Research Report*; IHS: London, UK; April 2012.

[9] Borruso, A.V. *High-Density Polyethylene Resins - Chemical Economics Handbook (CEH) Marketing Research Report*; SRI Consulting: Menlo Park, CA; June 2011.

[10] Devanney, M. *Low-Density Polyethylene Resins - Chemical Economics Handbook (CEH) Marketing Research Report*; IHS Markit: London, UK; May 2012.

[11] Borruso, A. *Polypropylene Resins - Chemical Economics Handbook (CEH) Marketing Research Report*; SRI Consulting: Menlo Park, CA; August 2011.

[12] Devanney, M. *Vinyl Chloride Monomer-Chemical Economics Handbook (CEH) Marketing Research Report*; SRI Consulting: Menlo Park, CA; February 2012.

[13] Kim, T.; Benavides, P.T.; Kneifel, J.D.; Beers, K.L.; Hawkins, T.R. Cross-Database Comparisons on the Greenhouse Gas Emissions, Water Consumption, and Fossil-Fuel Use of Plastic Resin Production and Their Post-Use Phase Impacts, *Resources, Conservation & Recycling*, 2023, 198, 107168. DOI: 10.1016/j.resconrec.2023.107168.

[14] Young, B.; Hawkins, T.R.; Chiquelin, C.; Sun, P.; Gracida-Alvarez, U.R.; Elgowainy, A. Environmental Life Cycle Assessment of Olefins and By-product Hydrogen from Steam Cracking of Natural Gas Liquids, Naphtha, and Gas Oil, *Journal of Cleaner Production*, 2022, 359, 131884. DOI: 10.1016/j.jclepro.2022.131884.

[15] Gracida-Alvarez, U.R.; Xu, H.; Benavides, P.T.; Wang, M.; Hawkins, T.R. Circular Economy Sustainability Analysis Framework for Plastics: Application for Poly(ethylene Terephthalate) (PET). *ACS Sustain. Chem. Eng.*, 2023, 11, 514-524. DOI: 10.1021/acssuschemeng.2c04626.

[16] *Cradle-to-Gate Life Cycle Analysis of High-Density Polyethylene (HDPE) Resin*; prepared by Franklin Associates for American Chemistry Council (ACC): Washington, D.C.; October, 2020.

[17] *Cradle-to-Gate Life Cycle Analysis of Olefins*; American Chemistry Council (ACC): Washington, D.C.; April, 2020.

[18] *Cradle-to-Gate Life Cycle Analysis of Low-Density Polyethylene (LDPE) Resin*; prepared by Franklin Associates for American Chemistry Council (ACC): Washington, D.C.; April, 2020.

[19] Wang, M.; Elgowainy, A.; Lee, U.; Bafana, A.; Banerjee, S.; Benavides, P.T.; Bobba, P.; Burnham, A.; Cai, H,; Gracida-Alvarez, U.R.; Hawkins, T.R.; Iyer, R.K.; Kelly, J.C.; Kim, T.; Kingsbury, K.; Kwon, H.; Li, Y.; Liu, X.; Lu, Z.; Ou, L.; Siddique, N.; Sun, P.; Vyawahare, P.; Winjobi, O.; Wu, M.; Xu, H.; Yoo, E.; Zaimes, G.; Zang, G. Summary of Expansions and Updates in GREET 2021; ANL/ESD-21/16; Argonne National Laboratory: Lemont, IL; October, 2021.

[20] Ye, L.; Qi, C.; Hong, J.; Ma, X. Life cycle assessment of polyvinyl chloride production and its recyclability in China, *Journal of Cleaner Production*, 2017, 142, 2965-2972. DOI: 10.1016/j.jclepro.2016.10.171.

[21] Keoleian, G.; Miller, S.; De Kleine, R.; Fang, A.; Mosley, J. *Life Cycle Material Data Update for GREET Mode*l; CSS12-12; Center for Sustainable Systems at University of Michigan: Ann Arbor, MI; July, 2012.

[22] Intergovernmental Panel on Climate Change IPCC 2022: Agriculture, Forestry and Other Land Uses (AFOLU). Climate Change 2022: Mitigation of Climate Change. Contribution of Working Group III to the Sixth Assessment Report of the Intergovernmental Panel on Climate Change [P.R. Shukla, J. Skea, R. Slade, A. Al Khourdajie, R. van Diemen, D. McCollum, M. Pathak, S. Some, P. Vyas, R. Fradera, M. Belkacemi, A. Hasija, G. Lisboa, S. Luz, J. Malley, (eds.)]. Cambridge University Press, Cambridge, UK and New York, NY, USA. doi: 10.1017/9781009157926.009.

[23] Gan Y.; Lu, Z.; He, X.; Hao, C.; Wang, Y.; Cai, H.; Wang, M.; Elgowainy, A.; Przesmitzki, S.; Bouchard, J.; Provincial Greenhouse Gas Emissions of Gasoline and Plug-in Electric Vehicles in China: Comparison from the Consumption-Based Electricity Perspective, *Environ. Sci. Technol.*, **2021**, 55, 6944–6956. DOI: 10.1021/acs.est.0c08217.

[24] World Energy Statistics and Balances 2022; International Energy Agency (IEA): Paris, France. https://www.iea.org/data-and-statistics/data-product/world-energy-statistics-and-balances (accessed on 12/15/2023).

[25] Electricity Information 2022; International Energy Agency (IEA): Paris, France. https://www.iea.org/reports/electricity-information-overview (accessed on 12/15/2023).

[26] Greenhouse Gas Emissions from Energy 2022; International Energy Agency (IEA): Paris, France. https://www.iea.org/data-and-statistics/data-product/greenhouse-gas-emissions-from-energy (accessed on 12/15/2023).

[27] Gan, Y.; El-Houjeiri, H.M.; Badahdah, A.; Lu, Z.; Cai, H.; Przesmitzki, S.; Wang, M. Carbon footprint of global natural gas supplies to China. *Nature Communications*, **2020**, 11, 824. DOI: 10.1038/s41467-020-14606-4.

[28] Global Methane Tracker 2022; International Energy Agency (IEA): Paris, France. https://www.iea.org/reports/global-methane-tracker-2022 (accessed on 12/15/2023).

[29] Natural Gas Information 2022; International Energy Agency (IEA): Paris, France. https://www.iea.org/reports/natural-gas-information-overview (accessed on 12/15/2023).

[30] Devanney, M.T. *Ethylene - Chemical Economics Handbook (CEH) Marketing Research Report*; SRI Consulting: Menlo Park, CA; July 2011.

[31] Giacobbe, G.B. *Propylene - Chemical Economics Handbook (CEH) Marketing Research Report*; SRI Consulting: Menlo Park; August 2011.

[32] *Dimethyl Terephthalate Market Forecast to 2032*; Reports and Data: Pune, India; 2023.

[33] Sesto, B.; Yoneyama, M. *Dimethyl Terephthalate (DMT) and Terephthalic Acid (TPA) - CEH Marketing Research Report*; SRI Consulting: Menlo Park, CA; August 2010.

[34] Lopez, G.; Keiner, D.; Fasihi, M.; Koiranen, T.; Breyer, C. From fossil to green chemicals: sustainable pathways and new carbon feedstocks for the global chemical industry, *Energy & Environmental Science*, 2023. DOI: 10.1039/d3ee00478c.

[35] Gracida-Alvarez, U.R.; Benavides, P.T.; Lee, U.; Wang, M. Life-cycle analysis of recycling of post-use plastic to plastic via pyrolysis. *Journal of Cleaner Production*, 2023, 425, 138867.

[36] The European Council of Vinyl Manufacturer (ECVM) website, https://pvc.org/about-pvc/vinyl-chloride-monomer-vcm-production/ (accessed on 11/16/2023).

[37] The S&P Global website, https://www.spglobal.com/commodityinsights/en/ci/products/vinyl-chloride-monomer-chemical-economics-handbook.html (accessed on 11/16/2023).

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