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Research Article

The Impact of Feedstock Availability on Defossilizing the Production of Chemical Building Blocks

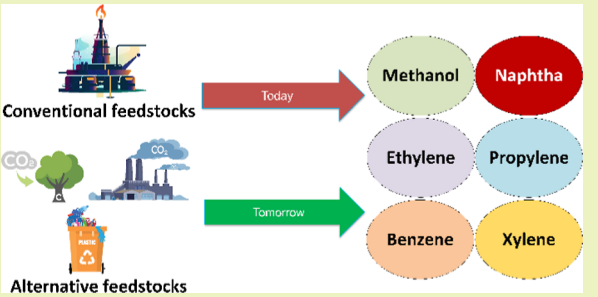
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Cite This: *ACS Sustainable Chem. Eng.* 2026, 14, 11530−11546

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ABSTRACT: Alternative carbon sources (ACSs) such as CO_2, biomass, and plastic waste can be used to defossilize chemical building blocks (CBBs) such as methanol, olefins, and aromatics. While the existing literature estimates the quantities of ACSs to replace fossil fuel in specific processes, hubs, or areas, this work adds to the current state of the art by evaluating the impact of ACS feedstock availability on the portfolio of technologies that can be deployed to defossilize an existing petrochemical cluster. A superstructure-based multiobjective optimization model of the Port of Rotterdam was run with eight novel ACS-based processes to evaluate the impact of defossilizing CBB production. The paper explicitly evaluates the performance of the cluster using the following performance indicators: amount of feedstock use, byproduct production, CAPEX, electricity demand, water demand, and change in the minimum selling price of the products. Three cases are analyzed: the fossil-based cluster and two cases, one with unlimited and one with limited feedstock availability. The results show that if feedstocks are considered unlimited, plastic waste-based pyrolysis, methanol-to-olefin, and methanol-to-aromatics routes appear to be the most promising technologies. However, when feedstock constraints are included in the model, a combination of ACS and fossil-based technologies is required to meet product demand, and the level of defossilization significantly decreases. This research underscores the critical need to balance technological choices and realistic assessments of ACS feedstock availability to ensure a sustainable and economically viable transition of the chemical industry.



KEYWORDS: *defossilization, feedstock limitation, feedstock availability, olefins, aromatics, petrochemical cluster, technology portfolio*

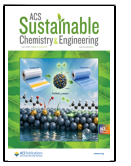
INTRODUCTION

Day-to-day essentials like packaging, cosmetics, medicines, fertilizers, detergents, paints, and fuels are made from fossil-based raw materials such as crude oil or natural gas.[1] In order to reach ambitious CO_2 emission reduction targets needed to mitigate climate change, replacing the use of fossil-based feedstocks with sustainable carbon feedstocks (hereafter defossilization) will be vital.[1]

In today's petrochemical industry, fossil-based raw materials such as crude oil or natural gas are first broken down into chemical building blocks (CBBs) such as carbon monoxide, methanol, ethylene, propylene, benzene, and xylene before further processing (see Figure 1). These CBBs are the backbone of the chemical sector. They can be defossilized by using alternative carbon sources (ACSs) such as CO_2, biomass, and plastic waste as feedstocks. Despite the increasing interest, several studies[2−8] have raised concerns about current and future ACS availability. In a study by the Royal Society[7] aiming to identify the challenges of defossilizing the chemical industry, it was estimated that globally, 7000 Mt of sustainable biomass (wet) will be needed for a net-zero emission from the chemical industry;[7] but only 4300 Mt biomass (wet) is available globally (as of 2022).[7] A similar picture has been reported at the European level. For instance, Bazzanella and Ausfelder[9] estimated that by 2050, Europe will need around 250 Mt of dry biomass (30% of the available sustainable and non-food-based biomass in Europe).[9] In the context of chemical production, sustainable biomass refers to organic materials derived from forestry, agriculture, or waste (such as lignocellulosic residues, municipal organic waste, manure, algae, and waste lipids) that can be used for the production of chemicals and fuels, which lowers net greenhouse gas emissions without compromising food security, animal feed availability, land-use, biodiversity, and soil protection.[10−12]

Regarding the availability of plastic waste feedstock, low recycling rates, contamination, and high energy intensity of waste-to-chemical processes are the main challenges identified from the literature.[7] Currently, approximately 300 to 400 Mt of plastic are produced globally, and only about 9% are recycled,

Received: December 17, 2025
Revised: May 29, 2026
Accepted: June 1, 2026
Published: June 15, 2026



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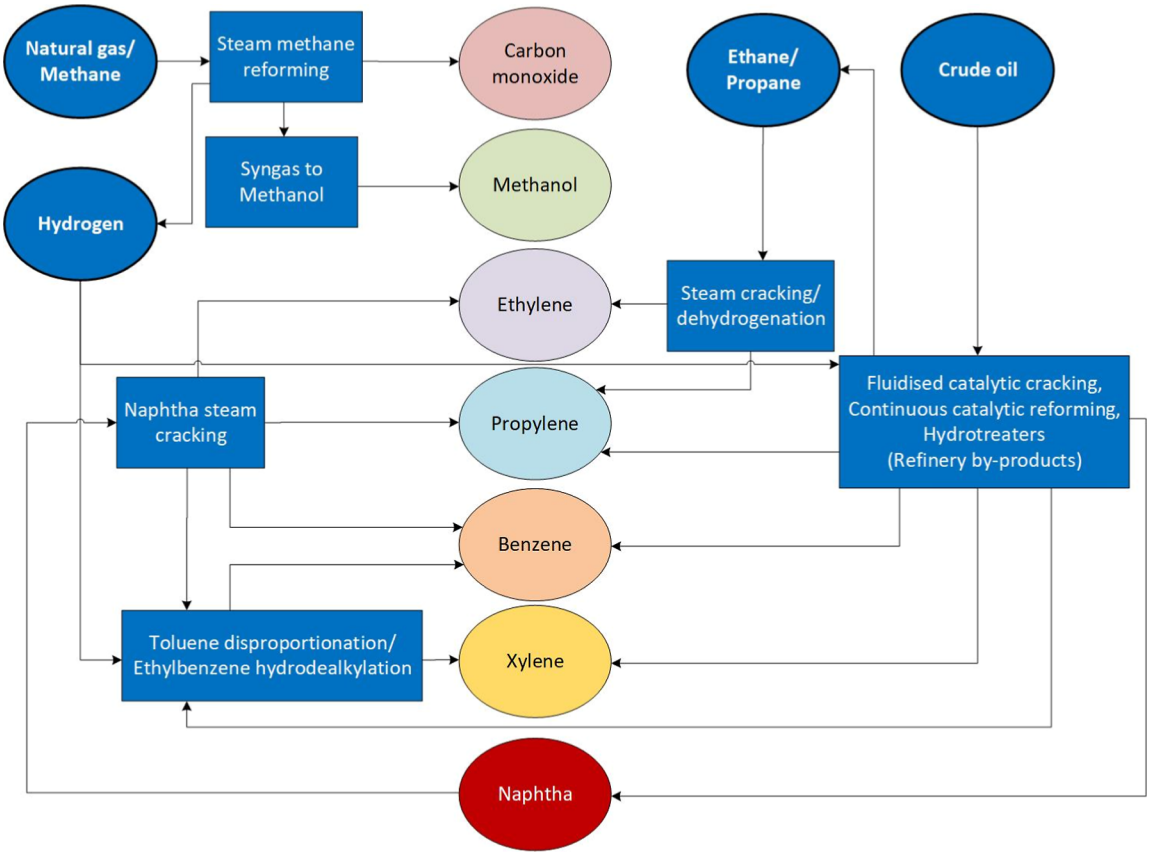


Figure 1. Overview of fossil-based feedstocks and technologies typically used for the production of chemical building blocks.

raising questions about the feedstock availability for waste-to-chemical processes. For plastic waste feedstock, most studies[7,9,13] do not provide an estimate of the required feedstock; however, they report that Europe produces around 49 Mt of plastics, of which only about 10% (~5 Mt) is recycled, and the rest is lost as export, stockpile, misclassified waste, unsorted waste, landfill, and for energy recovery.[13]

For CO_2 feedstock, a study by the Royal Society[7] estimated a CO_2 demand of 2800 Mt to 4700 Mt, which is less than 1% of the annual anthropogenic CO_2 emissions in 2022 (~59000 Mt CO_2).[7] However, as indicated by Lopez et al.,[3] the main challenge for CO_2-based chemical production is the large energy requirement for direct electrochemical reduction or hydrogen production. The authors estimated that around 30000 TWh to 40000 TWh of electricity will be required to satisfy the CO_2-based global chemical sector. Currently, about 30000 TWh of electricity is generated globally (as of 2023),[14] which means that an additional electricity equivalent to current global production will be required for a CO_2-based chemistry transition. Bazzanella and Ausfelder[9] estimated that by 2050, Europe will need around 4900 TWh of green electricity (140% of the projected available supply) and 300 Mt of CO_2 feedstock (corresponding to c.a. 80% of large source emissions).

Zanon-Zotin et al.[4] estimated that with limitations on alternative feedstocks and renewable electricity availability, only about 28% of the global primary chemical sector could be defossilized.[4] Similarly, Bertrams et al.[8] studied the potential of ACSs for the transition of the Port of Rotterdam (PoR) and estimated that biomass, bio-oils, plastic waste, and pyrolysis oil could only replace up to 40% of the total carbon feedstock demand in the PoR industrial cluster. The study[8] did not make explicit how the limit was calculated, but they indicated that the low feedstock replacement was due to the lower energy densities of ACS feedstocks and conversion efficiencies of ACS technologies compared to fossil-based counterparts.[8] In addition, ACS-based technologies are currently at a low technology readiness level (TRL), leading to higher CAPEX and lower energy efficiencies compared to the fossil-based counterparts. These studies[4,8] do not address how feedstock availability affects the technology deployment and performance of the cluster, which is a main limitation to understanding deployment. As identified by Samadi et al.,[15] defossilizing a highly integrated petrochemical cluster can impact its performance because of changes in energy, product portfolios, investments, and ACS feedstock availability.[15]

Even though such studies[4,5,7−9,16] provide valuable insights into the amount of ACSs required or the limit up to which the chemical sector can be defossilized, they do not take into account existing processes, conditions, and geographical limitations of today's petrochemical clusters and usually assume greenfield conditions. To date, top-down studies[8,15,16] in the literature do not quantify how feedstock defossilization could impact the performance of an industrial cluster. This work contributes to the current state of the art by evaluating the impact of ACS feedstock availability on investment requirements and the technology portfolio of a highly interconnected petrochemical cluster through bottom-up analysis. The paper aims to assess how limitations in feedstock and energy could change the deployment of technologies for defossilzsing CBB production and consequently the performance of existing petrochemical clusters. The analysis uses the

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following indicators: amount of carbon feedstock use, byproduct production, CAPEX, electricity demand, water demand, and changes to minimum selling prices to assess the performance change in the cluster.

METHODOLOGY

A superstructure-based multiobjective optimization model was used to explore optimal technology portfolios under different feedstock availability cases for defossilizing CBB production in a petrochemical cluster. The selected CBBs were methanol, ethylene, propylene, benzene, and *p*-xylene. Fossil feedstocks considered in the reference case were carbon monoxide, methanol from natural gas and propylene, C4's, naphtha, pygas, reformate from oil, while the defossilization cases considered CO_2, biomass, and plastic waste as ACSs. These three ACSs allow recycling of carbon already present in the technosphere and biosphere, directly reducing the need for new fossil extraction. Other ACS feedstocks like municipal organic waste, manure, algae, or waste lipids were not considered as biochemical processes were not part of the preselected technologies for CBB production. Both the fossil and ACS-based technologies were modeled in Aspen Plus v12 with capacities and product purities mimicking CBB production in the Port of Rotterdam (PoR), The Netherlands. The PoR is part of the largest chemical cluster zone in Europe (the Antwerp−Rotterdam−Rhein−Ruhr economic zone), which is responsible for 30% to 40% of the chemical production in Europe.[17] The energy, mass, and investment data obtained from the Aspen Plus models mimicking the CBB production in the PoR were used in the optimization model for the technology portfolio analysis.

Optimization Model

The optimization model used has been reported in Tan et al.[18,19] and includes a multilayered graph representation of energy, mass, and equipment (capital expenditure—CAPEX) data.[19] The model is described in detail for the reference case. For this work, two objective functions (eq 1) were defined to find the optimal technology portfolio that (a) minimizes the amount of fossil carbon used for CBB production and (b) maximizes the use of existing assets in the cluster as companies are likely to try to use assets that are already in place.

The amount of fossil carbon used in the cluster ($Carbon_{Fossil}^{Import}$) was calculated as the sum of carbon in fossil-based feedstocks FM_{FC} (see eq 2), i.e., in carbon monoxide, methanol, propylene, C4s, naphtha, pygas, reformate, and natural gas. To maximize the use of existing assets and minimize new investments, eq 3 was used, where a CAPEX penalty was defined as the sum of investments required for the new ACS technologies plus the loss of existing CAPEX as a consequence of dismantling fossil-based processes.

$$\min(\mathrm{Carbon}_{\mathrm{Fossil}}^{\mathrm{Import}}, \mathrm{CAPEXpenalty}) \tag{1}$$

$$\mathrm{Carbon}_{\mathrm{Fossil}}^{\mathrm{Import}} = \sum_{f \in FM_{\mathrm{FC}}} \mathrm{Feed}_f^{\mathrm{Mass}} \times m_f^{\mathrm{Carbon}} \tag{2}$$

$$\mathrm{CAPEXpenalty} = \Big(\sum_{p \in PP_{Fossil}} (1 - p_p^I) \times CAPEX_p + \sum_{p \in PP_{\mathrm{ACS}}} p_p^I \times \mathrm{CAPEX}_p \Big) \tag{3}$$

where f is the carbon feedstock; FM_{FC} is the set of fossil-based carbon feedstock; $Feed_f^{\mathrm{Mass}}$ is the mass flow of the inlet carbon feedstock f; m_f^{Carbon} is the mass fraction of carbon in the fossil-based feedstock f; p is the CBB production process, which can use either fossil or alternative carbon sources; PP_{Fossil} is the set of fossil-based processes; PP_{ACS} is the set of ACS-based processes; p_p^I is the integer value representing the number of plants per process p; and CAPEX_p is the total capital expenditure required for process p.

In the model, two constraints were applied. First, the same amount of final products had to be produced as in the reference case (fossil feedstock-based case) (see eq 4), with an upper demand margin of 20% (1.2 in eq 4) and 10% of operational margin (denoted as operational flexibility, K_p^{Flex}; see eq 5). Second, the maximum amount of feedstock available could not be surpassed (eq 6); the limitations are given in the feedstock Availability section below. Equation 4 therefore ensures that the CBB demand in the considered cluster is always met, while eq 5 provides a marginal flexibility for the CBB production processes to account for the discrete nature of the optimization solutions, and finally, eq 6 limits the quantity of ACS feedstock available for CBB production.

$$(1 - K_d^{\mathrm{Tol}}) \le \frac{\mathrm{Mass}_{d,cc}^{\mathrm{Out}}}{X_{d,cc}^{\mathrm{Demand}}} \le 1.2 \qquad \forall\, d \in D, \forall\, cc \in CC \tag{4}$$

$$\left(1 - \frac{K_p^{\mathrm{Flex}}}{10^4}\right) \times p_p^I \times K_{p,cc}^{\mathrm{Cap}} \le \mathrm{Mass}_{p,cc}^{\mathrm{Out}} \le p_p^I \times K_{p,cc}^{\mathrm{Cap}} \quad \forall\, p \in PP_{\mathrm{ACS}} \cap PP_{\mathrm{Fossil}}, \forall\, cc \in CC \tag{5}$$

$$\mathrm{Feed}_f^{\mathrm{Mass}} \le \mathrm{Limit}_{\mathrm{ACS}} \qquad \forall\, f \in \mathrm{FM}_{\mathrm{ACS}} \tag{6}$$

where K_d^{Tol} is the tolerance parameter of the lower demand constraint; $\mathrm{Mass}_{d,CC}^{\mathrm{Out}}$ is the mass flow of the product of the demand node d; $X_{d,cc}^{\mathrm{Demand}}$ is the reference case production rate of each CBB, CC is the set of chemical building blocks, and cc is the chemical building block; D is the set of demands of each chemical building block and d is the demand of each chemical building block; K_p^{Flex} is the operational flexibility parameter of process p; $K_{p,cc}^{\mathrm{Cap}}$ is the nominal production capacity of component cc of process p; and f is the carbon feedstock, $\mathrm{FM}_{\mathrm{ACS}}$ is the set of ACS-based carbon feedstock, $\mathrm{Feed}_f^{\mathrm{Mass}}$ is the mass flow of the inlet carbon feedstock, and $\mathrm{Limit}_{\mathrm{ACS}}$ is the alternative carbon feedstock limit.

The optimization model was run for three cases: the reference case (Case 1), a case with unlimited availability of ACS feedstock (Case 2), and a case with limited ACS feedstock availability (Case 3). The reference case was run to obtain the CAPEX, inlet fossil carbon, product flows, and energy needs of the fossil-based cluster. For Case 2, only eqs 4 and 5 were used as constraints because in this case, there are no ACS feedstock constraints, while for Case 3, eqs 4−6 were used to include limits on ACS feedstock availability in the assessment. The optimization model was solved using the augmented ε-constraint method, which generated a set of technology portfolio solutions as a Pareto front for each case.[19] From the Pareto front, using eq 7, the solutions that achieved 55%, 75%, and 95% defossilization of CBBs with a deviation of ±1% were selected (for Case 2 and Case 3) and are discussed in this work. These defossilization targets were chosen to analyze the impact of ambitious targets. The 55% limit aligns

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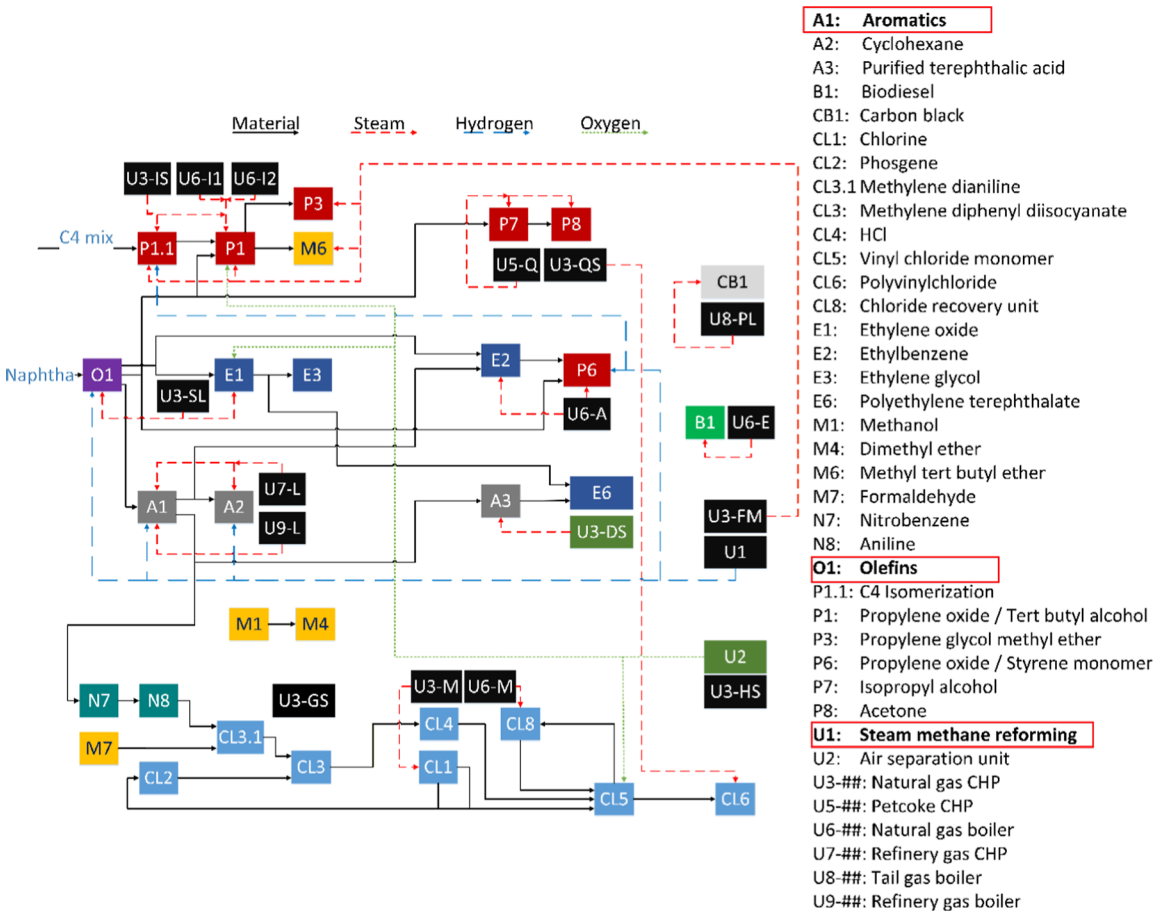


Figure 2. Simplified diagram of the petrochemical cluster used as the reference case. The diagram presents the main mass and energy flows. The red boxes show the CBB production considered in this study. (Abbreviations: CHP—combined heat and power plant).

with the EU Fit for 55 package to reduce the net greenhouse gas emissions by at least 55% by 2030, while the upper limit of 95% was set based on the maximum amount that can be defossilized when there are no feedstock limits found in the previous work.[20]

$$\text{Defossilization\%} = \frac{\text{Carbon(ref)}^{\text{Import}}_{\text{Fossil}} - \text{Carbon}(i)^{\text{Import}}_{\text{Fossil}}}{\text{Carbon(ref)}^{\text{Import}}_{\text{Fossil}}} \times 100 \quad (7)$$

where $\text{Carbon(ref)}^{\text{Import}}_{\text{Fossil}}$ is the fossil-based carbon entering into the cluster for the reference case and $\text{Carbon}(i)^{\text{Import}}_{\text{Fossil}}$ is the fossil-based carbon entering into the cluster when using the ACS-based technologies in Cases 2 and 3.

The technology portfolios were compared using six key performance indicators (KPIs), namely, percentage of defossilization (eq 7), CAPEX penalty (eq 3), amount of feedstocks usage (eq 6), mass flows of byproducts (eq 4), energy needs (eq 8), and average minimum selling price of each CBB (eq 10). The energy need was calculated as the net utility flow of the CBB production processes, as given in eq 8.

$$\text{Energy need} = \sum_{p \in PP_{\text{ACS}} \cap PP_{\text{Fossil}}} \text{Mass}^{In}_{p,cc} \times X^{\text{Demand}}_{p,cu} - \text{Mass}^{In}_{p,cc} \times X^{\text{Supply}}_{p,cu} \; \forall \; cu \in CU \quad (8)$$

where CU is the set of utilities considered, $\text{Mass}^{In}_{p,cc}$ is the component stream (i.e., for example, ethylene in the case of naphtha cracker) on which the process streams are linearized, cu is the utility type, $X^{\text{Supply}}_{p,cu}$ is the specific energy production with respect to the limiting component $\text{Mass}^{In}_{p,cc}$ for process p and utility cu, and $X^{\text{Demand}}_{p,cu}$ is the specific energy need with respect to the limiting component $\text{Mass}^{In}_{p,cc}$ for process p and utility cu.

The average selling price of each CBB was calculated from its minimum selling price (MSP) using eqs 9 and 10, assuming a payback period of 12 years.

$$\sum_{cc \in CC} \text{Mass}^{\text{Out}}_{p,cc} \times \text{MSP}_{p,cc} = \frac{\text{CAPEX}}{\text{Payback period}} + \text{OPEX} \; \forall \; p \in PP_{\text{ACS}} \cap PP_{\text{Fossil}} \quad (9)$$

$$\text{MSP}_{cc} = \frac{\sum_{p \in PP_{\text{ACS}} \cap PP_{\text{Fossil}}} \text{Mass}^{\text{Out}}_{p,cc} \times \text{MSP}_{p,cc}}{\sum_{p \in PP_{\text{ACS}} \cap PP_{\text{Fossil}}} \text{Mass}^{\text{Out}}_{p,cc}} \; \forall \; cc \in CC \quad (10)$$

Fossil-Based Cluster (Reference Case)

This study takes as a point of departure the petrochemical cluster in the PoR, The Netherlands, which is part of the Antwerp−Rotterdam−Rhein−Ruhr chemical cluster zone in Europe.[17] The reference cluster in this study includes 57 chemical processes and their utility islands, which were

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Table 1. Reference Case Technologies for Chemical Building Block Production (Detailed Data and Assumptions of the Process Models Are Provided in the Zenodo Repository, as Given in the Supporting Information and the Associated Content Section)

Chemical	Technology	Design Basis			
		Capacity	Feedstock	Reactor	Downstream Processing
Hydrogen	Steam methane reformer (SMR)	118 kt/y hydrogen	Natural gas (71% methane)	Steam reforming at 850 °C, 17 bar	Pressure swing adsorption
Methanol	Steam methane reformer (SMR)	90 kt/y methanol	Natural gas (71% methane)	Steam reforming at 900 °C, 20 bar; Syngas to methanol at 255 °C, 70 bar	High pressure distillation
Olefins	Naphtha steam cracker (NSC)	878 kt/y ethylene and 497 kt/y propylene	Full range naphtha	Steam cracking at 850 °C, 5 bar	Cryogenic distillation
Aromatics	Aromatics distillation (AD)	892 kt/y benzene and 754 kt/y *p*-xylene	Pygas and reformate	Toluene disproportionation at 400 °C, 30 bar; Xylene isomerization at 400 °C, 14 bar	Extractive distillation

modeled in Aspen Plus v12.[18] The modeling assumptions, bibliographic sources, material, energy, and cost data for the reference case petrochemical cluster are reported in the Supporting Information. The reference cluster is described in detail in Tan et al.'s work.[18,19]

The main mass flows in the reference case are shown in Figure 2.[18] It includes the naphtha steam cracker (NSC) for the production of ethylene, propylene, and benzene (O1 in Figure 2); aromatics distillation (AD) for the production of benzene and *p*-xylene (A1 in Figure 2); and the steam methane reformer (SMR) for the production of hydrogen (U1 in Figure 2). All processes were designed to produce products with 99.5 wt % purity. As the design basis, we considered the technical specifications shown in Table 1. All process model details (block diagrams, input data, assumptions, references and model results) are provided in a Zenodo repository, as given in the Associated Content. 2018 was used as the base year; plant life was assumed to be 25 years, located in The Netherlands (Rotterdam). In the reference case, the carbon feedstocks imported for CBB production were carbon monoxide, methanol, propylene, C4s, naphtha, pygas, reformate, and natural gas. Even though propylene and C4s were produced in the cluster in the NSC process, approximately 20% of the total propylene demand and 75% of the total C4s demand in the cluster are met by imports. The reference case included the following utilities: low−low pressure steam (LLPS), low pressure steam (LPS), medium pressure steam (MPS), high pressure steam (HPS), high−high pressure steam (HHPS), cooling water (CW), refrigerants, high temperature (HT) utility, and electricity, as detailed in the Supporting Information (Table S1).

Ex-Ante ACS Technologies

Eight ACS-based pathways (see Table 2) for the production of methanol, ethylene, propylene, benzene, and *p*-xylene were selected and analyzed in this study. The eight ACS-based pathways were selected based on a first-principles technology prescreening methodology described in previous studies.[21,22] Potential ACS technologies were modeled in Aspen Plus v12, as described in previous studies.[21,22] The ACS-based processes were modeled to produce methanol, ethylene, and benzene in the range of 400−415 kt/y, 300−330 kt/y, and 530−540 kt/y, respectively. The production range was selected to meet at least 1/3rd demand of olefins and aromatics in the reference petrochemical cluster, which is ambitious for ACS-based technologies while still being industrially relevant to achieve economies of scale. To meet additional demand, the model has the option to deploy more than one plant.

Two green hydrogen plants, water electrolysis-small (WE-S) and water electrolysis-large (WE-L), with hydrogen production capacities of 17 kt/y and 110 kt/y, respectively, were used to provide the required hydrogen for the selected ACS-based processes. Two different production scales were selected for the green hydrogen plants to provide flexibility for the optimization model to install smaller capacity plants when the hydrogen demand is lower, thereby avoiding over-production and to ensure economies of scale when the hydrogen demand is higher. The green hydrogen-based plants were mainly required for the hydrogenation process steps in the CO_2- or biomass-based processes as these feedstocks have a zero (for CO_2) or low hydrogen to carbon mole ratio (H/C of 1.7) compared to the fossil-based feedstocks (H/C of 4 and 2.2 for methane and naphtha, respectively). The CAPEX for hydrogen production is included in the optimization model, as required by the defossilized cluster. The descriptions, block flow diagrams, mass balances, energy balances, and CAPEX of the processes are provided in Supporting Information Section 2, Figures S1 to S12, and Tables S2 to S14. The detailed data set for each process model can be found in the Zenodo repository, as indicated in the Supporting Information and in the Associated Content.

Feedstock Availability

ACS feedstock limitations were assumed based on the reported availability of these feedstocks in The Netherlands. Given the importance of the transition, when possible, the upper limit was selected. Although CO_2 availability is not limited as it could be obtained from the atmosphere via direct air capture, the amount of renewable energy needed to use this feedstock is limited. Using a renewable electricity generation limit of 200 PJ/y,[23] which is in line with the expected electricity use by the Dutch industry in a 2030−2050 scenario,[24] a CO_2 feedstock limit of 3 Mt/y was estimated. A biomass supply limit of 8 Mt/y in The Netherlands was assumed based on Rabou et al.[25] (see Table S15 for a detailed breakdown of biomass types and quantities). The estimated plastic waste collection in The Netherlands is about 1.9 Mt/y,[26] while the total production of plastics is estimated to be 6.2 Mt/y.[28] This large difference between production and collection is due to about 3.8 Mt/y of plastic being exported to outside The Netherlands, and only about 2.3 Mt/y is used locally.[27] Based on this, a municipal plastic waste (MPW) limit of 2 Mt/y was assumed. Also, considering the global plastic waste trade of 12 to 6 Mt/y[29] and a plastic waste generation of 30 Mt/y[29] in the EU 28 + 2 (see Supporting Information Table S16), an additional plastic waste source, sorted plastic waste (SPW) with a limit of 5 Mt/y, was assumed in the study.

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Table 2. Selected ACS-Based Technologies for Chemical Building Block Production (Detailed Data and Assumptions of the Process Models Are Provided in the Zenodo Repository, as Given in Supporting Information and the Associated Content Section)

Chemical	Technology	Design Basis			
		Capacity	Feedstock	Reactor	Downstream processing
Hydrogen	Water electrolysis (WE)	17 kt/y hydrogen (WE-S); 110 kt/y hydrogen (WE-L)	Water	Proton exchange membrane electrolyzer at 80 °C, 1.02 bar	Flash drum, molecular sieve
Methanol	CO_2 hydrogenation to methanol (CM)	406 kt/y methanol	Food grade CO_2	Hydrogenation reactor at 255 °C, 70 bar	High-pressure distillation
	Biomass steam gasification to syngas + syngas to methanol (BM)	414 kt/y methanol	Wood pellet	Steam gasifier at 830 °C, 2 bar; Hydrogenation reactor at 255 °C, 70 bar	Solid−gas separation, tar removal, acid gas cleaning, cryogenic distillation, high-pressure distillation
	Plastic waste steam gasification to syngas + syngas to methanol (PM)	408 kt/y methanol	Municipal plastic waste (Netherlands)	Steam gasifier at 900 °C, 1.02 bar; Hydrogenation reactor at 255 °C, 70 bar	Solid−gas separation, tar removal, high-pressure distillation
Olefins	Direct electrochemical reduction of CO_2−H_2O to ethylene (CO)	329 kt/y ethylene	Food grade CO_2	Steam cracking at 80 °C, 1.1 bar	Molecular sieve, cryogenic distillation
	Biomass steam gasification to syngas + syngas to Fischer−Tropsch and methanol + methanol to olefin (BO)	301 kt/y ethylene and 298 kt/y propylene	Wood pellet	Steam gasifier at 830 °C, 2 bar; Fischer−Tropsch at 340 °C, 30 bar; Hydrogenation reactor at 255 °C, 70 bar; Methanol to olefin at 450 °C, 30 bar	Solid−gas separation, tar removal, acid gas cleaning, cryogenic distillation
	Plastic waste low-temperature pyrolysis (PLTP) + Naphtha steam cracking (NSC)	303 kt/y ethylene and 172 kt/y propylene	Sorted plastic waste (Deutsche Kunststoff recycling 329 and Deutsche Kunststoff recycling 324)	Pyrolysis reactor at 420 °C, 1.02 bar; Steam cracking at 850 °C, 5 bar	Vacuum distillation, cryogenic distillation
	Methanol-to-olefins (MO)	314 kt/y ethylene and 398 kt/y propylene	Methanol	Methanol-to-olefin at 450 °C, 30 bar	Solid−gas separation, cryogenic distillation
Aromatics	methanol-to-aromatics (MA)	535 kt/y benzene and 972 kt/y *p*-xylene	Methanol	Methanol-to-aromatics at 450 °C, 60 bar; Toluene disproportionation at 400 °C, 30 bar; Xylene isomerization at 400 °C, 14 bar	Solid−gas separation, cryogenic distillation, extractive distillation

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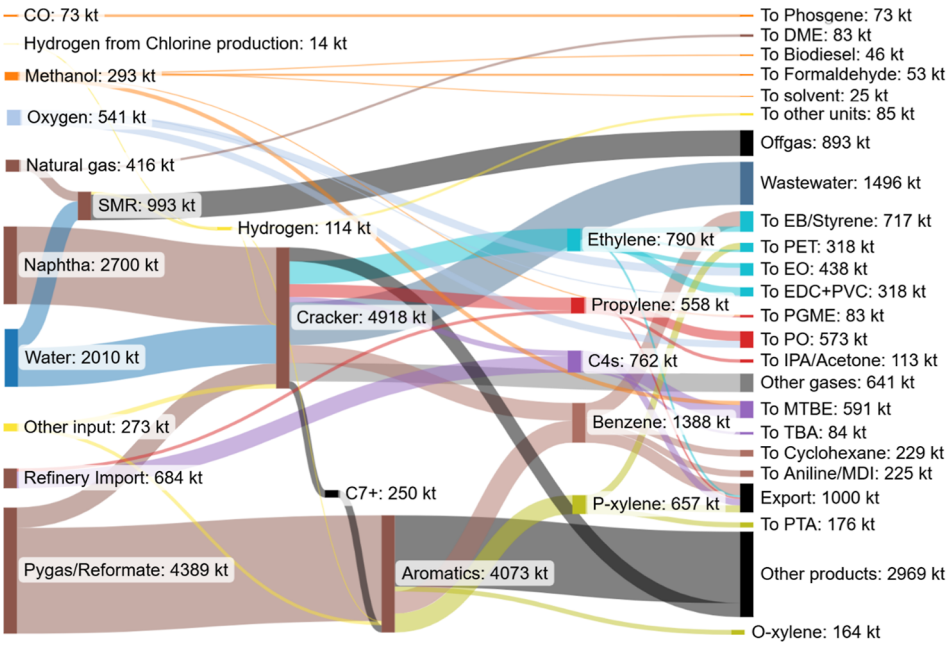


Figure 3. Sankey diagram of mass flows per year for Case 1 (Abbreviations: EO—ethylene oxide, EDC—ethylene dichloride, DME—dimethyl ether, PVC—polyvinyl chloride, PET—polyethylene terephthalate, EB—ethylbenzene, PO—propylene oxide, PGME—propylene glycol methyl ether, IPA- iso-propyl alcohol, MTBE—methyl *tert*-butyl ether, TBA—*tert*-butyl alcohol, MDI—methylene diphenyl diisocyanate, PTA—purified terephthalic acid, and SMR—steam methane reformer).

Table 3. Portfolio of Technologies, CAPEX, Mass Flows, Energy Flows, and Average Minimum Selling Price of CBB in Case 1 (Reference Case)[a]

Case	Technologies (number of units)	CAPEX (billion EUR)	Fossil feedstocks (kt/y)	Alternative feedstocks (kt/y)	Energy needed or produced (PJ/y)	CBB production (kt/y)	Average minimum selling price (EUR/t)
Reference case	Hydrogen: 1 SMR	2	CO: 73	CO_2: 0	LLPS: 0.2	Ethylene: 790	Ethylene: 1075
	Methanol: imported fossil methanol		Methanol: 293	Biomass: 0	LPS: 11	Propylene: 558	Propylene: 1000
	Naphtha: imported fossil naphtha		Propylene: 110	SPW: 0	MPS: 10	Benzene: 1388	Benzene: 884
	Olefin: 1 NSC		C4:574	MPW: 0	HPS: −0.3	*p*-Xylene: 657	*p*-Xylene: 1105
	Aromatics: 1 AD		Naphtha: 2700		HHPS: −1.5		
			Pygas: 2334		HT: 4.2		
			Reformate: 2055		Electricity: 7		
			Natural gas: 416		CW: 48		

[a]The negative sign (−) refers to heat production and the positive sign (+) refers to cooling, heating, or electricity needs in the energy needed or produced column (abbreviations: SMR: steam methane reformer, NSC: naphtha steam cracker, AD: aromatics distillation, SPW: sorted plastic waste, MPW: municipal plastic waste, CBB: chemical building block, LLPS: low−low pressure steam, LPS: low pressure steam, MPS: medium pressure steam, HPS: high pressure steam, HHPS: high−high pressure steam, HT: high temperature, and CW: cooling water).

RESULTS AND DISCUSSION

Case 1 (Reference Case)

In the reference case, about 7.2 Mt/y of fossil carbon is required in the cluster as feedstock to produce approximately 3.4 Mt/y of CBB for the different value chains considered in this study. As seen in Figure 3, the import of naphtha, pygas, and reformate for olefin and aromatic production accounts for 86% of the inlet fossil carbon flow in the cluster. In the reference case, 100% of the methanol demand (293 kt/y) is met by imports. Natural gas is used for the production of gray hydrogen and DME. The highest amounts of waste and byproducts come as heavy hydrocarbons (2969 kt/y from the aromatics plant) and as off-gases (893 kt/y from the steam methane reformer and 641 kt/y from the olefins plant). Around 114 kt/y of hydrogen, 1.3 Mt/y of olefins, and 2 Mt/y of aromatics are produced in the reference cluster. As shown in Table 3, aromatics constitute the highest CBB production, accounting for 60% of the CBB mass flow in the clusters. In terms of water demand, 1.3 Mt/y is used by the naphtha steam cracker, and 0.7 Mt/y is used by the steam methane reformer. The aromatic plant does not need external water.

In the reference case, the considered CAPEX includes a naphtha steam cracker (1.1 billion EUR), an aromatics distillation unit (0.7 billion EUR), and a steam methane reformer (0.3 billion EUR). Thus, even though aromatics account for the highest production, the most expensive contribution comes from the olefin production plant. This is due to the higher complexity of the olefins plant compared to the aromatics plant. The olefins plant contains a high-temperature cracker (~850 °C) and a complex high pressure cryogenic (~30 bar and −88 °C) based distillation train, while the aromatics plant consists of a medium-temperature disproportionation reactor (~400 °C) and a moderately

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Table 4. Portfolio of Technologies, CAPEX Penalty, Mass Flows, Energy Flows, and Average Minimum Selling Price for Case 2 (Defossilization without Feedstock Limitations)[a]

Defossilization target	Technologies (number of units)	CAPEX penalty (billion EUR)	Fossil feedstocks (kt/y)	Alternative feedstocks (kt/y)	Energy needed or produced (PJ/y)	CBB production (kt/y)	Average minimum selling price (EUR/t)
Hydrogen: 1 SMR		10.8	CO:73	CO_2: 0	LLPS: 0	Ethylene: 811	Ethylene: 1107
Methanol: 14 PM + fossil methanol import			Methanol: 3489	Biomass: 0	LPS: 11	Propylene: 540	Propylene: 1157
Naphtha: 2 PLTP + fossil naphtha import			Propylene: 24	SPW: 10000	MPS: −24	Benzene: 1156	Benzene: 1434
Olefin: 1 NSC			C4:518	MPW: 4340	HPS: −76	*p*-Xylene: 972	*p*-Xylene: 2445
Aromatics: 1 MA			Naphtha: 600		HHPS: −1.5		
			Pygas: 335		HT: 38		
			Reformate: 375		Electricity: 23		
			Natural gas: 315		CW: 91		
75%	Hydrogen: 1 SMR	14.5	CO: 73	CO_2: 0	LLPS: 0	Ethylene: 811	Ethylene: 1113
	Methanol: 23 PM		Methanol: 0	Biomass: 0	LPS: 27	Propylene: 540	Propylene: 1184
	Naphtha: 2 PLTP + fossil naphtha import		Propylene: 24	SPW: 10000	MPS: −37	Benzene: 1156	Benzene: 1535
	Olefin: 1 NSC		C4:518	MPW: 7130	HPS: −81	*p*-Xylene: 972	*p*-Xylene: 2679
	Aromatics: 1 MA		Naphtha: 600		HHPS: −1.5		
			Pygas: 335		HT: 61		
			Reformate: 375		Electricity: 30		
			Natural gas: 315		CW: 114		
95%	Hydrogen: 2 WE-S	33	CO: 73	CO_2: 0	LLPS: 0	Ethylene: 2221	Ethylene: 2512
	Methanol: 63 PM		Methanol: 0	Biomass: 0	LPS: 146	Propylene: 2851	Propylene: 2376
	Naphtha: 0		Propylene: 0	SPW: 0	MPS: −91	Benzene: 1093	Benzene: 2072
	Olefin: 7 MO		C4:518	MPW: 19531	HPS: −39	*p*-Xylene: 972	*p*-Xylene: 2707
	Aromatics: 1 MA		Naphtha: 0		HHPS: 0		
			Pygas: 0		HT: 158		
			Reformate: 0		Electricity: 65		
			Natural gas: 0		CW: 242		

[a]The negative sign refers to heat production and the positive sign refers to cooling, heating, or electricity needs (abbreviations: SMR: steam methane reformer, NSC: naphtha steam cracker, PM: plastic waste to methanol, PLTP: plastic waste low temperature pyrolysis, MO: methanol to olefin, MA: methanol to aromatics, WE-S: water electrolysis-small, SPW: sorted plastic waste, MPW: municipal plastic waste, CBB: chemical building block, LLPS: low−low pressure steam, LPS: low pressure steam, MPS: medium pressure steam, HPS: high pressure steam, HHPS: high−high pressure steam, HT: high temperature, and CW: cooling water).

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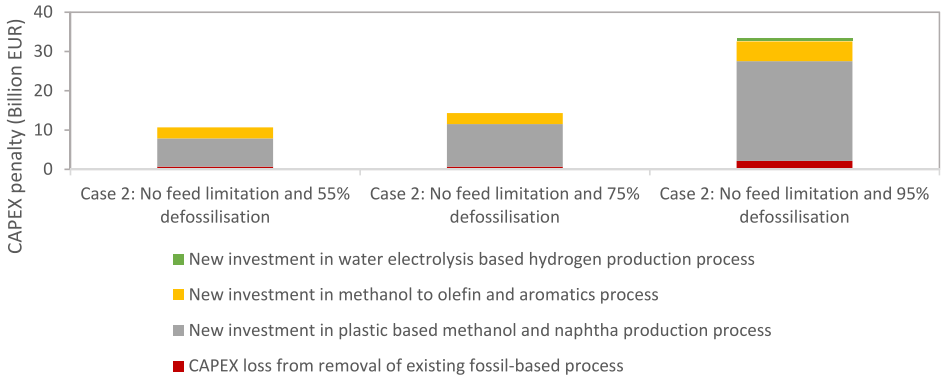


Figure 4. Breakdown of CAPEX penalty in Case 2 for 55%, 75%, and 95% defossilization targets.

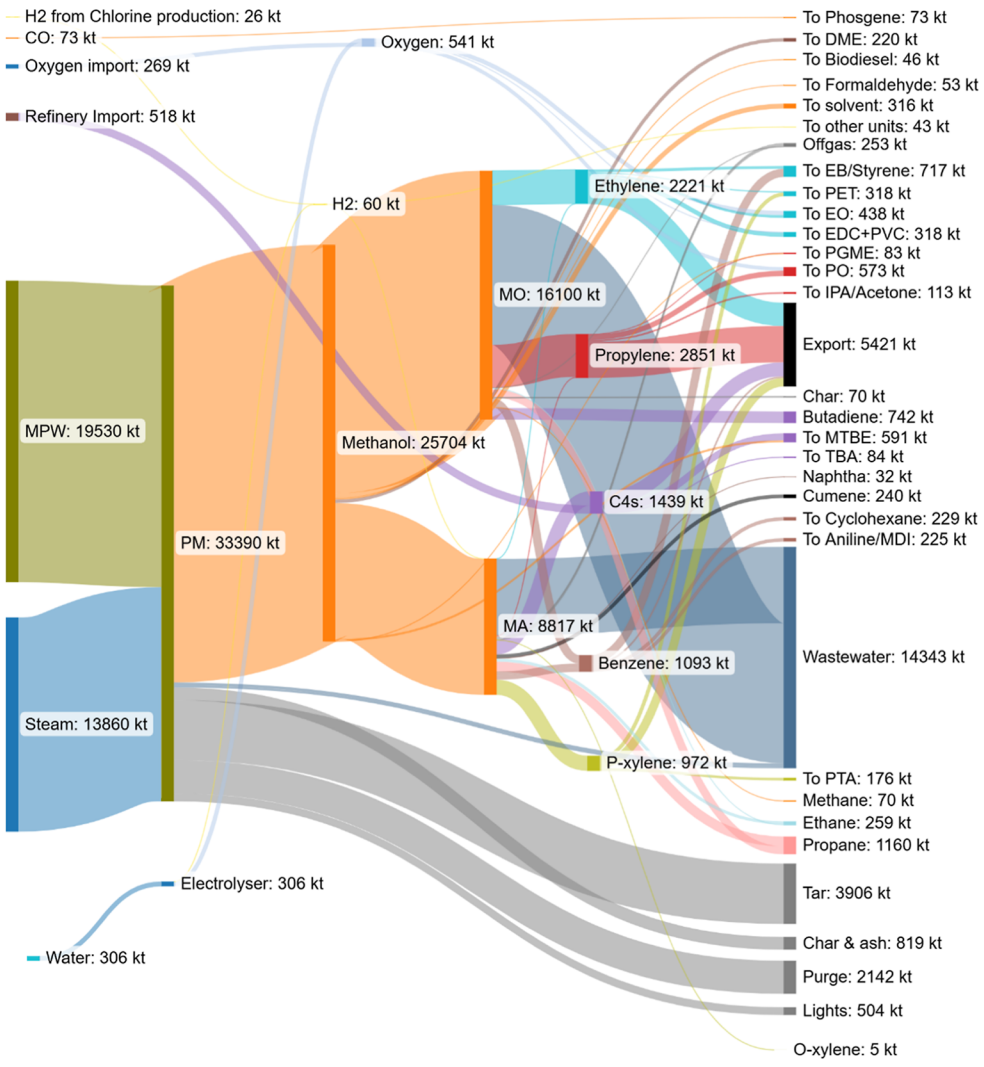


Figure 5. Sankey diagram of mass flows per year for the selected ACS-based processes in Case 2 and the 95% defossilization target (abbreviations: PM—plastic waste to methanol, MA—methanol to aromatics, VGO—vacuum gas oil, SPW—sorted plastic waste, MPW—municipal plastic waste, EO—ethylene oxide, EDC—ethylene dichloride, DME—dimethyl ether, PVC—polyvinyl chloride, PET—polyethylene terephthalate, EB—ethylbenzene, PO—propylene oxide, PGME—propylene glycol methyl ether, IPA—iso-propyl alcohol, MTBE—methyl *tert*-butyl ether, TBA—*tert*-butyl alcohol, MDI—methylene diphenyl diisocyanate, PTA—purified terephthalic acid, and SMR—steam methane reformer).

complex (azeotropic and vacuum) distillation train. This results in higher CAPEX for olefins than for aromatics. The average selling prices of the methanol, olefins, and aromatics calculated from the model are around 650 EUR/t, 1000 EUR/t , and 880−1100 EUR/t, respectively.

In terms of energy, out of the 7 PJ/y electricity needed for the CBB production plants in the cluster, 6.6 PJ/y is used by the naphtha steam cracker and about 85% of it is for the cryogenic-based high-pressure product distillation section. All of the CBB production routes are endothermic due to the

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cracking and reforming reactions involved. However, off-gases are combusted to produce 15 PJ of steam. This reduces the steam needs from 31 PJ to around 16 PJ in the cluster.

Case 2 (Defossilization without Limitations on Feedstock Availability)

The multiobjective optimization resulted in the Pareto fronts shown in the Supporting Information (Section S4 in Figure S14). As shown in Table 4, the deployment of the ACS-based processes results in up to 95% defossilization in Case 2, by reducing the total amount of fossil carbon from 7.2 Mt to 0.5 Mt, using about 19.5 Mt of plastic waste. Regardless of the defossilization target, the results show that technologies that use plastic waste as feedstock are selected in all cases (reaching up to 95% defossilization), while CO_2- or biomass-based technologies are not part of the technology portfolio. This is because when it is assumed that there are no limits in feedstock availability, the model selects the technology with the lowest CAPEX to fulfill the demand for CBB production. Among the three ACS feedstocks, the plastic-waste-based technologies have the lowest CAPEX per tonne of product.

Plastic waste-based technologies show the lowest CAPEX penalty per tonne of product as they require the least amount of external hydrogen due to the better C/H/O ratio of plastic waste compared to biomass and CO_2 feedstocks. For instance, to produce 400 kt of methanol, the plastic-waste-based methanol process requires around 403 MEUR of CAPEX, while the biomass- and CO_2-based methanol processes need 2050 million EUR and 2903 million EUR, respectively. This high CAPEX for CO_2 and biomass-based technologies is mostly due to the hydrogen requirements; hydrogen production through water electrolysis contributes about 46% and 86% of the inside battery limit-related CAPEX for biomass- and CO_2-based processes, respectively. As seen in Figure 4, the major share of the CAPEX penalty due to defossilization in Case 2 is accounted for by the plastic waste feedstock to methanol (i.e., plastic waste steam gasification followed by syngas to methanol) and naphtha (i.e., plastic waste pyrolysis) production processes due to their high cost of implementation. The CAPEX loss from the removal of existing fossil-based processes accounts for only 6% of the CAPEX penalty.

In the 55% defossilization scenario, the amount of fossil carbon used in the cluster is reduced by fully replacing the fossil-based production of aromatics (benzene, *p*-xylene) with an ACS-based methanol-to-aromatics process and by partially defossilizing the olefin production using synthetic naphtha produced through the plastic waste-based pyrolysis route. In this scenario, 78% of naphtha is produced from the plastic-waste-based pyrolysis process, which requires around 10 Mt of sorted plastic waste. For comparison, the global plastic waste trade is about 8 to 14 Mt.[28] In addition to the sorted plastic waste, about 4 Mt of municipal plastic waste is required in this scenario for the production of methanol. Thus, substantial quantities of plastic waste (14 Mt), equivalent to those available in the global trade, would be required in this scenario.

The 55% and 75% defossilization scenarios have the same technology portfolio (see in Supporting Information Figures S18 and S20 their technology portfolio), while the main difference is in the amount of methanol imported vs produced in the cluster (see Supporting Information Figures S18−S21). In the 55% defossilization scenario, about 3.5 Mt of fossil-based methanol is imported, while in the 75% defossilization scenario, all the required methanol is produced inside the cluster. This additional methanol production inside the cluster (i.e., 3.5 Mt of methanol) leads to an extra demand of 2.8 Mt of municipal plastic waste and 2 Mt of water. In the 55% and 75% defossilization scenarios, it can be observed that due to the selection of the plastic waste pyrolysis process, high quantities of byproducts like diesel and vacuum gas oil are produced. These heavy hydrocarbons could be further cracked using heavy-oil cracking technologies[30] or sent to oil refineries for processing as synthetic fuels, which can defossilize other unintended sectors. These options could provide further defossilization in the cluster but are not included in this study.

The highest percentage of defossilization (95% scenario) is only achieved by removing the naphtha cracker (see Supporting Information Figures S22 and 5) as the refinery inputs like pygas or reformate can only be curtailed by shutting down the unit. The second major change observed in the technology portfolio is that only in the 95% defossilization scenario, the model deploys water electrolyzers for hydrogen production, while in the other scenarios, the cluster still operates with the fossil-based steam methane reformer. This is because the plastic waste-based processes require comparatively less additional hydrogen due to the better C/H ratio of 1:2 in the plastic waste feedstock. For instance, the methanol to aromatics and the plastic waste pyrolysis units in the 55% and 75% scenarios need around 49 kt of hydrogen compared to the reference case production of 114 kt. Thus, the existing hydrogen plant in the cluster could absorb the new hydrogen demand in these defossilization scenarios.

In the 95% defossilization scenario, the CBB production of ethylene and propylene is significantly higher than in the reference case (see Figure 5 and Supporting Information Figure S18). The production of ethylene and propylene increases by 2.7 and 5.3 times, respectively, compared with current production processes. This is due to the difference in the ethylene-to-propylene production ratio of the naphtha cracker in the reference case (equal to 0.6) and the methanol-to-olefin plants in Case 2 (1.3), leading to a high overshoot in propylene production. This effect is not present in the 55% and 75% scenarios as olefins are produced using plastic waste pyrolysis followed by the existing naphtha cracking process, resulting in a similar share of olefins as in the reference case. Regarding aromatic production, this overshoot is not observed for benzene and/or *p*-xylene productions (see Figure 5), even though the benzene to *p*-xylene ratio is 1 and 0.55 for the reference case and Case 2, respectively (i.e., more *p*-xylene is produced in the ACS case than in the reference case).This is because in the ACS case, benzene can be produced from both the methanol-to-aromatics and methanol-to-olefin plants, and the model selects a combination of these technologies to fulfill the benzene demand. Such a technology combination is selected because the CAPEX of the methanol-to-olefin process is around 2.2 billion EUR, while the CAPEX of the methanol-to-aromatics process is 2.8 billion EUR to produce 500 kt of benzene. Hence, as in the model, it is cheaper to produce benzene via the methanol-to-olefin route; about 50% of the benzene demand is met with the methanol-to-olefins process, and the other 50% is produced with the methanol-to-aromatics process. Although it is cheaper to produce benzene with the methanol-to-olefin process, the methanol-to-aromatics process is selected as it is the only process that produces xylene among the considered technologies. Thus, the methanol-to-aromatics process (the most expensive process) is first selected to meet

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the xylene demand, which also produces benzene; however, as all the benzene demand is not fully covered, the methanol-to-olefin process (the cheaper process) is deployed to cover the remaining benzene demand. Such trends are the result of CAPEX penalty optimization criteria in the objective function in the model. In addition to the target CBB products, significant quantities of light gases like ethane, propane, and C4s are also produced in the ACS case (see Figure 5), which could open new synergies and product lines in the petrochemical cluster to improve material utilization efficiencies.

In terms of the average selling price of each CBB for each defossilization scenario, Table 4 shows that the plastic waste pyrolysis-based olefin process results in the least price change impact to its selling prices, increasing between 3% and 18% compared to the fossil case, depending on the plastic waste-based process used. The methanol-to-olefin and aromatic processes create a price increase between 60% and 145% based on the amount of fossil-based methanol imported and the ACS-based methanol produced in the cluster (fossil-based methanol at 650 EUR/t is cheaper than the plastic waste-based methanol at 860 EUR/t).

Defossilizing the petrochemical cluster results in a notable change in water demand and wastewater production in the cluster (see Figure 3 for Case 1, Supporting Information Figure S19 for Case 2 with 55% defossilization, Supporting Information Figure S21 for Case 2 with 75% defossilization, and Figure 5 for Case 2 with 95% defossilization). Compared to the reference case (2 Mt of water needed for the naphtha steam cracker and steam methane reformer), between 3 and 14 Mt of additional water is needed, mainly due to the plastic waste steam gasification process. Even for the 95% defossilization scenario, the water needed for the electrolysis-based hydrogen production process is only 0.3 Mt (to produce 34 kt hydrogen) compared to the 14 Mt required for the steam gasification process. Hence, in Case 2, considerable water stress is created on the cluster due to the steam gasification process. Also, about a 4 to 10 times increase in wastewater production is observed in the ACS-based case compared to that in the reference case. Thus, water recycling will be critical to reduce water stress due to the use of the selected ACS-based technologies.

In general, the results of this case highlight that the role of methanol in the cluster increases with defossilization, from 293 kt/y methanol in the reference case to 9.2 Mt/y in the 55% (or 75%) scenario and 26 Mt/y in the 95% defossilization scenario, where methanol is used as the intermediate chemical for olefin and aromatic production.

Case 3 (Defossilization with Limited Feedstock Availability)

In Case 3, the solutions in the Pareto front only reached 55% defossilization (see Supporting Information Figure S15) due to ACS feedstock limitations, compared to the 95% defossilization reached in Case 2. A combination of ACS and fossil-based feedstocks became necessary to meet the CBB demand in the cluster, when the alternative feedstock is limited (see Table 5). To achieve 55% defossilization, the CAPEX penalty in Case 3 is 2.3 billion EUR higher than in the 95% defossilization scenario in Case 2 (see Figure 6 and Supporting Information Figure S27 for the detailed breakdown of CAPEX penalty). Around 48% of the CAPEX penalty is due to the installation of water electrolyzers required for hydrogen production. Due to

Table 5. Portfolio of Technologies, CAPEX Penalty, Mass Flows, Energy Flows, and Average Minimum Selling Price for Case 3 (Defossilization with Feedstock Limitations)[a]

Defossilization	Technologies (number of units)	CAPEX penalty (billion EUR)	Fossil feedstocks (kt/y)	Alternative feedstocks (kt/y)	Energy needed or produced (PJ/y)	CBB production (kt/y)	Average minimum selling price (EUR/t)
55%	Hydrogen: 6 WE-S + 6 WE-L	35.3	CO: 73	CO_2: 2400	LLPS: 3	Ethylene: 811	Ethylene: 1169
	Methanol: 9 μB + 6 PM + 3 CM + Fossil methanol import		Methanol: 1760	Biomass: 7741	LPS: −21	Propylene: 540	Propylene: 1430
	Naphtha: 1 PLTP + Fossil naphtha import		Propylene: 24	SPW: 5000	MPS: −13	Benzene: 1156	Benzene: 2437
	Olefin: 1 NSC		C4:518	MPW: 1860	HPS: −61	*p*-Xylene: 972	*p*-Xylene: 4759
	Aromatics: 1 MA		Naphtha: 1650		HHPS: −1.5		
			Pygas: 335		HT: 15		
			Reformate: 375		Electricity: 199		
			Natural gas: 115		CW: 141		

[a]Note: the negative sign refers to heat production and the positive sign refers to cooling, heating or electricity needs (abbreviations: NSC: naphtha steam cracker, BM: biomass to methanol, CM: CO_2 to methanol, CO: CO to ethylene, PM: plastic waste to methanol, PLTP: plastic waste low-temperature pyrolysis, MA: methanol to aromatics, WE-S: water electrolysis-small, WE-L: water electrolysis-large, SPW: sorted plastic waste, MPW: municipal plastic waste, CBB: chemical building block, LLPS: low−low pressure steam, LPS: low pressure steam, MPS: medium pressure steam, HPS: high pressure steam, HHPS: high−high pressure steam, HT: high temperature, and CW: cooling water).

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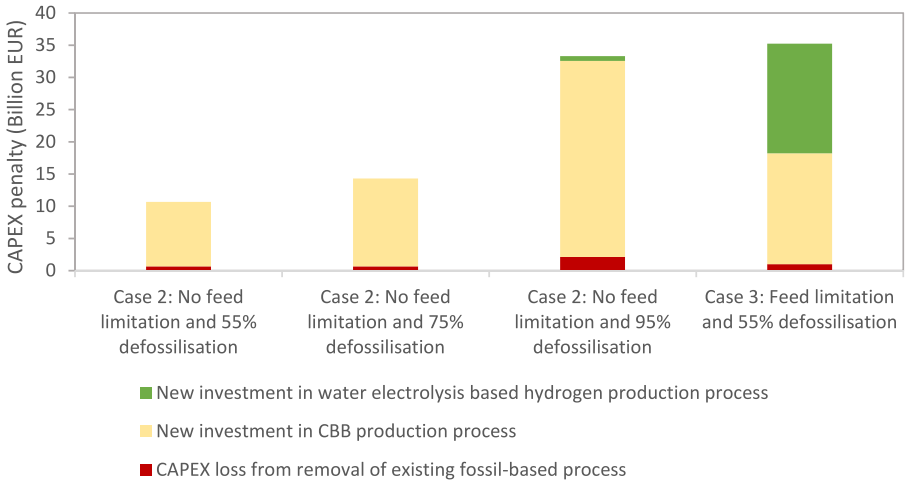


Figure 6. Comparison of the CAPEX penalty between Cases 2 and 3.

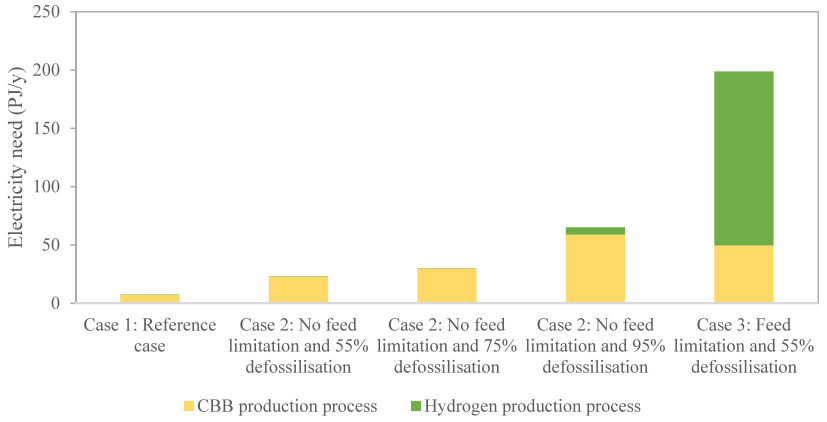


Figure 7. Comparison of the electricity needed in the different cases and scenarios.

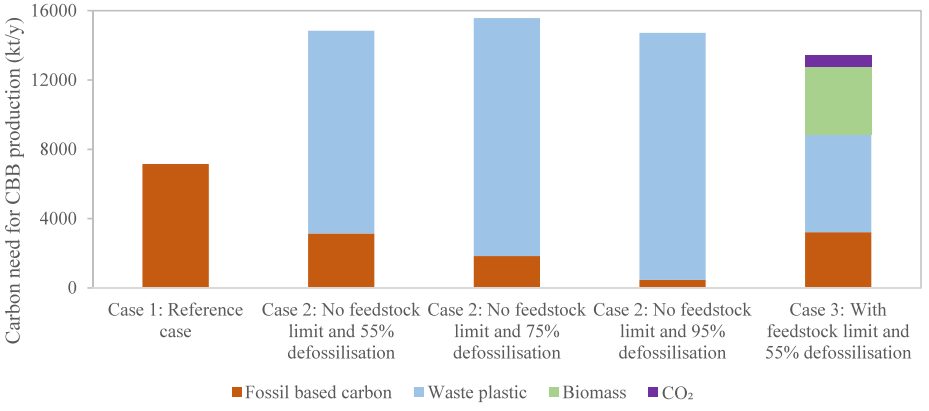


Figure 8. Comparison of carbon needed for CBB production in the different cases and scenarios.

plastic waste feedstock limitation, around 782 kt/y of hydrogen is required in Case 3 compared to 60 kt/y in the 95% defossilization scenario in Case 2. Furthermore, in Case 2, 63 plastic-waste-based methanol plants are installed, while in Case 3, only 6 use plastic waste and the rest of the methanol demand is met by other routes (9 plants using biomass and 3 plants using CO_2 as feedstock). Because of the use of hydrogen-based options, compared to Case 2 and as seen in Figure 6, an additional CAPEX is mainly needed for green hydrogen production. The removal of existing fossil-based technologies did not cause a significant contribution to the CAPEX penalty as only 6% of the total CAPEX penalty is due to the removal of existing technologies in Case 3.

The electricity consumption is also significantly changed; the electricity demand needed to achieve 55% defossilization in Case 3 is 3 times higher than in the 95% defossilization scenario in Case 2 and 28 times higher than the current consumption in the reference cluster (see Figure 7 and Supporting Information Figure S28 for detailed breakdown). In terms of feedstock (check Figure 8 and Supporting

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Information Figure S25 for a detailed breakdown of carbon feedstock), compared to the reference case, Cases 2 and 3 need approximately twice as much alternative carbon for defossilization due to the lower energy densities and higher byproduct or waste production in the ACS-based processes. Water demand is 1.7 times lower in Case 3 than in the 95% defossilization scenario in Case 2 (and 4 times higher than in the reference case). The water demand for the 95% defossilization scenario in Case 2 is higher than for the 55% defossilization scenario in Case 3 due to the higher need of a gasifying agent to produce more methanol to achieve higher defossilization. The water needed in Case 3 is higher than in the reference case due the higher steam dilution required in gasification compared to the naphtha cracker (i.e., steam/carbon feedstock ratio of 1 and 0.5, respectively, see Supporting Information Figure S26 for a detailed comparison of water demand in the three cases).

In Case 3, when the limit of 5 Mt/y of sorted plastic waste is included in the model as a constraint, only one plastic waste pyrolysis unit is selected, and thus, about 60% of the naphtha needed is still from a fossil-based origin (as seen in Figure 10).

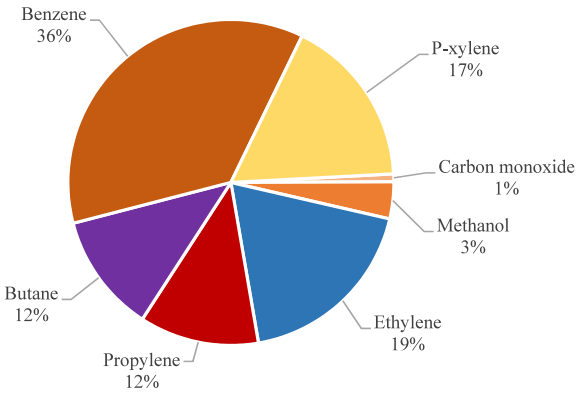


Figure 9. Embedded carbon distribution in the reference case petrochemical cluster (Note: the chart shows that benzene is the highest embedded carbon contributor, followed by ethylene, *p*-xylene, propylene, butane, methanol, and carbon monoxide).

The olefin production is only partially defossilized, and CBB production remains dependent on fossil-based feedstock to meet the demand of ethylene and propylene in the cluster. The methanol to olefin technology is not chosen in this case, which also leads to a similar ethylene to propylene production profile to that of the reference case, and overshoot of byproduct formation is avoided. Similarly, with limited availability of CO_2, biomass, and municipal plastic waste for methanol production, the model prefers to defossilize the aromatics process over the olefin process (see in Supporting Information Figure S24 the technology portfolio selected for Case 3 and 55% defossilization). This is because more than 50% of the embedded carbon in the CBB is accounted for by benzene and *p*-xylene (see in Figure 9 and Supporting Information Figure S16 the embedded carbon distribution in cluster products). Therefore, defossilizing aromatics creates the highest embedded carbon impact in the cluster. A total of 9.2 Mt/y methanol is needed for the methanol-to-aromatics plant; however, only 7.4 Mt/y methanol can be produced due to the ACS feedstock limitations. Hence, 20% of methanol required by the cluster is imported. Thus, in Case 3, the CBB production of olefins and aromatics is only partially defossilized, and the cluster still depends on fossil-based feedstocks to meet the CBB demand.

In case 3, the average selling price of CBB increased by 10−40% for olefins and by 175−330% for aromatics. The price change is lower for olefins than for aromatics as the most price-competitive plastic waste pyrolysis-based process is selected over the methanol-to-olefin route. The price change of aromatics is higher in Case 3 when compared to all scenarios in Case 2 due to the higher average methanol price (1568 EUR/t in Case 3 compared to 780−860 EUR/t in Case 2). This is because in Case 2, 100% of the methanol is obtained from the cheaper fossil-based and plastic waste-based routes, while in Case 3, 53% of the methanol is obtained from the more expensive CO_2- and biomass-based routes.

Note that the technology portfolios in this paper have been optimized for minimizing CAPEX penalty based on the current CAPEX and efficiencies of the selected ACS-based processes. The main limitations of the study are that the technology portfolio results based on the superstructure-based multi-objective optimization only take into account CAPEX penalty and other criteria like net CO_2 emissions are not considered in the assessment. Also, future technology improvements for low TRL technologies and the impact of byproduct or waste valorization on achievable defossilization targets were not analyzed. For example, it was assumed that a 30% stack replacement[31] is required for the CO_2 electrolyzer every 5 years.[32] The optimization method used in the study could be further improved by taking into account future technology improvements for the ACS-based processes, which could potentially change the technology portfolio over time.

CONCLUSIONS

Defossilizing the production of chemical building blocks (CBBs) like methanol, olefins, and aromatics, using alternative carbon sources (ACSs) like CO_2, biomass, and plastic waste, will be crucial for the transition of the chemical industry. Previous studies have pointed out that limited availability of ACS feedstocks will impact the technology portfolio selected for defossilizing the CBB production. However, the impact of the ACS feedstock availability on the technology portfolio and the performance of a brown field petrochemical cluster have not been studied in depth. In this research, to analyze and quantify the impact of feedstock availability on the performance of a cluster, three cases were considered mimicking the situation in the Port of Rotterdam: a reference case representing the current petrochemical cluster (Case 1), a case without limits on ACS availability (Case 2), and a case with limited ACS availability (Case 3). The technology portfolio in each case was selected based on an optimization model that minimizes fossil feedstock usage in the cluster and maximizes the use of existing assets in the cluster to achieve different percentages of defossilization compared to the reference case.

The results show considerable changes in the cluster performance in terms of carbon feedstock, byproduct production, CAPEX, electricity, water demand, and price change for Cases 2 and 3 compared to Case 1. In Case 2, when sufficient ACSs were considered available, the plastic waste pyrolysis (i.e., pyrolysis with steam cracking) and the plastic waste gasification-based processes (i.e., gasification with syngas to methanol, followed by methanol to olefin and methanol to aromatics) appeared to be the preferred choices due to their low CAPEX and low hydrogen needs. Up to 95% defossilization could be achieved in Case 2 for the production of the CBB, which required around 19.5 Mt/y of plastic waste

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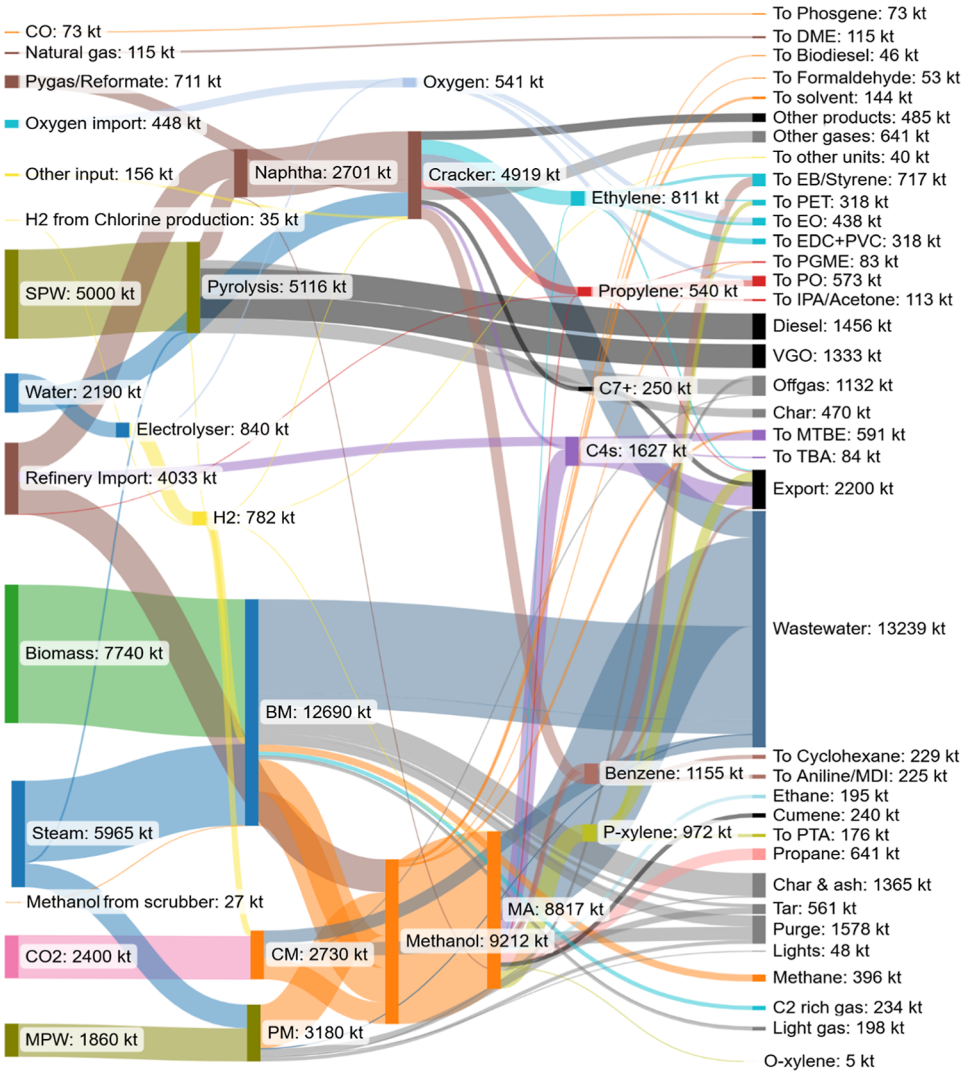


Figure 10. Material flow diagram per year for Case 3 (55% defossilization considering feedstock limitations) (abbreviations: BM—biomass to methanol, CM—CO_2 to methanol, PM—plastic waste to methanol, MA—methanol to aromatics, VGO—vacuum gas oil, SPW—sorted plastic waste, MPW—municipal plastic waste, EO—ethylene oxide, EDC—ethylene dichloride, DME—dimethyl ether, PVC—polyvinyl chloride, PET—polyethylene terephthalate, EB—ethylbenzene, PO—propylene oxide, PGME—propylene glycol methyl ether, IPA—iso-propyl alcohol, MTBE—methyl *tert*-butyl ether, TBA—*tert*-butyl alcohol, MDI—methylene diphenyl diisocyanate, PTA—purified terephthalic acid, and SMR—steam methane reformer).

(more than three times the current total plastic production in The Netherlands). This high ACS need was mainly due to the large byproduct production, such as off gas and heavy hydrocarbons (between 6 Mt/y and 12 Mt/y). A CAPEX penalty of approximately 33 billion EUR was incurred to achieve 95% defossilization in Case 2, with plastic waste conversion to the methanol intermediate accounting for about 76% of this CAPEX penalty. The electricity demand rose 9 times for the 95% defossilization scenario in Case 2 compared to Case 1 (i.e., 65 PJ/y, which is equivalent to 32% of total renewable energy production in The Netherlands in 2024) due to the high pressure needed in the methanol production process, particularly for syngas pressurization and recycling. The water demand in the 95% defossilization scenario in Case 2 was about 7 times higher than in Case 1, mainly due to the steam gasification process used in the methanol production process. The relevance of methanol as an intermediate for olefin and aromatic production increased in the 95% defossilization scenario in Case 2 as approximately 26 Mt/y of methanol was required compared to the 293 kt/y in Case 1. Thus, Case 2 shows that plastic-waste-based methanol-to-olefins and aromatics technologies are preferred routes because of the multiproduct nature, comparatively lower CAPEX, and lower hydrogen needs for defossilizing petrochemical clusters. However, a substantial amount of the feedstock is required.

In Case 3, the maximum defossilization obtained was 55% of the CBB production when considering ACS feedstock limits of 3 Mt/y of CO_2, 8 Mt/y of biomass, and 7 Mt/y of plastic waste. In this case, olefin production was partially defossilized by using synthetic naphtha from a plastic waste-based pyrolysis process; aromatic production was defossilized by using the methanol-to-aromatics process, and hydrogen production was defossilized by using water electrolysis. A comparison of the cases showed that high quantities of external hydrogen were required in Case 3, particularly for biomass and CO_2 feedstocks. Due to the high hydrogen demand, electricity demand was 28 times that in Case 1 (199 PJ/y, equivalent to the total renewable energy production in The Netherlands in

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2024). Furthermore, in Case 3, the cluster will incur around 35 billion EUR in investment to defossilize up to 55% of the cluster, which is about 18 times the CAPEX of the fossil-based CBB production plants. In Case 3, about 48% of the CAPEX penalty is due to the water electrolysis process for green hydrogen production. Case 3 highlights that in the case with limited ACS feedstock, the cluster operated by combining fossil-based and ACS-based technologies, namely, with 42% of carbon need met with plastic waste, 29% met with biomass, 24% met with fossil sources, and 5% met with CO_2. In such a case, assumptions about hydrogen production can significantly alter the required investment as it accounts for about 50% of the CAPEX penalty.

This research reaffirms that there is no silver bullet technology to defossilize the production of chemical building blocks and underscores the critical need to balance technological choices with realistic assessments of ACS feedstock availability to ensure a sustainable and economically viable transition for the chemical industry.

Future research can further explore the impacts of improving the defossilization potential in the ACS feedstock limited case by valorizing and recycling byproducts, off gases, and wastewater. Also, broader techno-economic assessment considering other ACS-based technologies, value chains, or clusters and conducting environmental assessments like life cycle analysis can be done to further strengthen evidence-based decision making for the transition of the petrochemical industry.

■ ASSOCIATED CONTENT

Data Availability Statement

The source code of the superstructure-based optimization can be found in Tan et al.[18,19]

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acssuschemeng.5c13309.

> Block flow diagrams, mass balances, energy balances, CAPEX data, and Pareto fronts for each case assessed in the study. Process models descriptions of fossil-based and ACS-based processes, containing modeling assumptions, mass balances, energy balances, economic data and bibliographic sources are provided in Zenodo as follows: Aromatics distillation: 10.5281/zenodo.14894694. Biomass steam gasification followed by Fischer−Tropsch and methanol-to-olefin: 10.5281/zenodo.14893888. Biomass steam gasification followed by syngas-to-methanol: 10.5281/zenodo.14894260. CO_2 hydrogenation to methanol: 10.5281/zenodo.14894463. CO_2−H_2O Direct electrochemical reduction to ethylene: 10.5281/zenodo.14894342. Methanol-to-aromatics conversion: 10.5281/zenodo.14894482. Methanol-to-olefin conversion: 10.5281/zenodo.14894523. Naphtha steam cracker: 10.5281/zenodo.14825234. Plastic waste pyrolysis followed by naphtha steam cracking: 10.5281/zenodo.14894590. Plastic waste steam gasification followed by syngas-to-methanol: 10.5281/zenodo.14894543 (PDF)

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Author Contributions

J. T. M, M. P−F., and A. R. R. conceptualized the paper. J. T. M modeled the Aspen Plus simulations, and M.T programmed the optimization model in Python. M. P−F and A. R. R. supervised the project. J. T. M. wrote the original draft. M.T, M. P−F, and A. R. R. reviewed and edited the manuscript. All authors discussed the results and commented on the manuscript.

Funding

This publication is part of the project *Unravelling the impacts of using alternative raw materials in industrial clusters* (grant number VI.C.183.010) financed by the Dutch Research Council (NWO).

Notes

The authors declare no competing financial interest.

■ ACKNOWLEDGMENTS

We thank Inna Stepchuk for her contribution to developing the reference case and Sebastian Quevedo for sharing the plastic waste to methanol Aspen Plus models, which were used for the assessment in this study.

■ ABBREVIATIONS

ACS	alternative carbon source
AD	aromatics distillation
BM	biomass to methanol
BO	biomass to olefins
CAPEX	capital expenditure
CBB	chemical building block
CHP	combined heat and power
CM	carbon dioxide to methanol
CO	carbon dioxide to ethylene
CW	cooling water
DME	dimethyl ether
EB	ethylbenzene
EDC	ethylene dichloride
EO	ethylene oxide
HHPS	high−high pressure steam
HPS	high pressure steam

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HT	high temperature
IPA	isopropyl alcohol
KPI	key performance indicator
LLPS	low−low pressure steam
LPS	low pressure steam
MA	methanol to aromatics
MDI	methylene diphenyl diisocyanate
MO	methanol to olefins
MPS	medium pressure steam
MPW	municipal plastic waste
MSP	minimum selling price
MTBE	methyl *tert*-butyl ether
NSC	naphtha steam cracking
OPEX	operational expenditure
PET	polyethylene terephthalate
PGME	propylene glycol methyl ether
PLTP	plastic waste low-temperature pyrolysis
PM	plastic waste to methanol
PO	propylene oxide
PoR	Port of Rotterdam
PTA	purified terephthalic acid
PVC	polyvinyl chloride
SMR	steam methane reforming
SPW	sorted plastic waste
TBA	*tert*-butyl alcohol
TRL	technology readiness level
VGO	vacuum gas oil
WE-L	water electrolysis-large
WE-S	water electrolysis-small

SYMBOLS

GW	gigawatt
Mt	million tonnes
kt	kilotonne
PJ	petajoule
MJ/kg	megajoule per kilogram
TWh	terawatt hour.

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