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EVALUATING THE TRANSITION OF THE PETROCHEMICAL INDUSTRY IN SPAIN TO CLIMATE NEUTRALITY BY 2050

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En memoria de Fernando Capelastegui (1930–2019)
Consejero y director general de Altos Hornos de Vizcaya

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RESUMEN DEL PROYECTO

El sistema energético mundial atraviesa su reconfiguración más profunda en un siglo. Impulsado por los objetivos climáticos y acuerdos internacionales, cada sector industrial se encuentra hoy en una pronunciada senda de descarbonización. La petroquímica—ya el mayor sumidero industrial de materias primas fósiles y una fuente creciente de CO₂—debe atender una demanda creciente de polímeros y, al mismo tiempo, recortar drásticamente sus emisiones.

Esta tesis desarrolla un modelo de optimización lineal de la industria petroquímica española para el período 2025-2050, integrando balances de masa y energía a nivel de proceso con costes de capital, operación y CO₂. La trayectoria de mínimo coste exige una implantación temprana y masiva de captura y almacenamiento de carbono (CCS) a lo largo de la cadena de valor, complementada—desde 2040—con la introducción selectiva de quemadores de hidrógeno verde en hornos de procesos específicos.

Palabras clave:

- Descarbonización
- Industria petroquímica
- Optimización lineal
- Transición hacia emisiones netas cero

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ABSTRACT

The global energy system is undergoing its most profound reconfiguration in a century. Driven by climate targets and international agreements, every industrial sector is now on a steep decarbonization trajectory. Petrochemicals—already the largest industrial sink for fossil feedstocks and a growing source of CO₂—must satisfy rising polymer demand while slashing emissions.

This thesis develops a bottom-up, linear-optimization model of Spain's petrochemical industry for 2025-2050, coupling process-level mass and energy balances with capital, operating and CO₂ costs. The least-cost pathway calls for early, large-scale deployment of carbon capture and storage (CCS) across the value chain, supplemented—from 2040 onward—by the selective introduction of green-hydrogen burners in selected process furnaces.

Keywords

- Decarbonization
- Petrochemical industry
- Linear optimization
- Net-zero transition

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Chapter 1. INTRODUCTION

Our current world energy system, largely based on the use of fossil fuels, has been evidenced to be unsustainable [1]. Almost nine years have gone by since the historic Paris agreement at COP21 in 2015, that set the goal to keep the rise in global surface temperature below 2 °C above pre-industrial levels. Decarbonization efforts, driven by international climate commitments, aim to bring carbon emissions to zero across various industrial sectors. The petrochemical industry, as one of the major consumers of fossil fuels, is also among the most challenging sectors to decarbonize due to its dependency on oil and gas feedstocks [2]. As shown by Figure 1, efforts to achieve climate neutrality have been widespread across most (over 90% by GDP) of the nations of the globe.

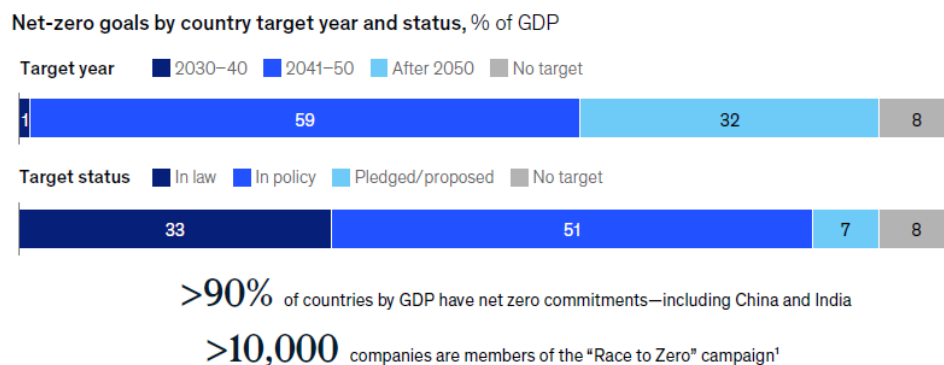


Figure 1 Decarbonization global progress [1]

Europe's green energy transition faces competitive pressure from policies such as the U.S. Inflation Reduction Act (IRA), which allocates \$370 billion to green energy investments [3]. The European Union's strategy to counteract these effects includes the Green Deal Industrial Plan aiming to increase Europe's manufacturing capacity in renewable technologies [4]. The pillars of this plan are:

- Simplified regulatory environment
- Faster access to funding
- Enhancing the EU workforces' skillset in renewable energy sectors

- Guarantee open trade to ensure resilient supply chains

While the progress during these past years has been considerable, with more than 2 TW of capacity installed globally in photovoltaic and wind power, more than 50 million electric and plug-in hybrid vehicles and over 100 million heat pumps installed, the rate of growth in these areas is not nearly enough to reach the 2050 net-zero goals set by the European Union [5]. It is estimated that only 10% of the necessary deployment of low-emissions technologies to reach net-zero has been achieved [5].

Spain's petrochemical industry is significant for the national economy, adding up to a total ca. €50 billion in revenues yearly [2]. Although oil product consumption has seen a slight decline, specific products like gasoline and kerosene have experienced increases. Spain also exports substantial amounts of refined products, positioning it as a net exporter within Europe. However, to align with Europe's broader decarbonization goals, the Spanish government is expected to adopt regulatory measures that promote sustainable industry practices while reducing reliance on imported fossil fuels [6].

Recently, in Spain, national plans to reduce emissions have been presented. In this context, the PNIEC¹ [6] is looking to reduce national emissions by 32% with respect to 1990s levels as well as having other secondary objectives such as a higher share of renewable energy production in the energy mix, an increase in final energy consumption efficiency, and reduction in energy dependency on other regions.

In this master's thesis, a method for evaluating the viability of the decarbonization of the Spanish petrochemical industry will be presented. To do this, linear optimization modelling tools will be used, following the lead of the already existing openMASTER model created by the Institute for Research in Technology (IIT) in the Pontifical University of Comillas (ICAI).

¹ In Spanish, *Plan Nacional Integrado de Energía y Clima* [National Energy and Climate Plan (NECP), in English].

1.1 GLOBAL ENERGY AND CLIMATE IMPERATIVE

Fossil fuels still provided 80 % of the world’s primary energy in 2023, and energy-related CO₂ emissions climbed again in 2024 to a record 37.8 Gt [7]. IEA’s World Energy Outlook 2024 shows that, even under today’s announced policies, coal, oil and gas demand merely plateau before 2030 rather than falling sharply [3].

At the same time, the remaining carbon budget compatible with a 1.5 °C pathway is vanishing [8]. Global greenhouse-gas output must fall 42 % by 2030 and 57 % by 2035; otherwise, the budget will be fully depleted around 2030 [8]. This information should be taken as a warning that without a near-term emissions peak “the 1.5 °C door will close.”

The geopolitical backdrop is also shifting. COP 28, which took place in Dubai in 2023, produced the first multilateral call to “transition away from fossil fuels”, signaling growing diplomatic pressure on hydrocarbon demand [9].

Yet the pace of clean-energy investment—about USD 1.7 trillion in 2023 versus the USD 4–5 trillion needed annually by 2030—remains insufficient. Bridging that gap will require deep decarbonization of hard-to-abate sectors, foremost among them petrochemicals.

1.2 WHY PETROCHEMICALS MATTER

The chemical and petrochemical value chain is already the largest industrial energy consumer and the third-largest source of direct industrial CO₂ emissions [3]. Unlike other industries, about 50 % of its fossil-fuel input is used as feedstock—carbon that ends up in products rather than being burned—so traditional fuel-switching or efficiency on their own cannot deliver net-zero.

Petrochemicals are also the single biggest growth driver of oil demand, the IEA projects they will account for more than one-third of oil-demand growth to 2030 and almost half to 2050 in its central outlook [3]. Demand for plastics, fertilizers and synthetic fibers is still rising rapidly in emerging economies, even as transport fuels start to peak.

These structural trends explain why most net-zero roadmaps rely on an integrated package of feedstock substitution (bio-, CO₂- or waste-based), process electrification, low-carbon hydrogen and large-scale CCUS to abate the sector—measures that are capital intensive and still in early deployment.

1.3 POLICY DRIVERS IN EUROPE AND SPAIN

The European Union’s response to the US Inflation Reduction Act (IRA)—which channels roughly USD 370 billion into clean-tech tax credits—is the Green Deal Industrial Plan (GDIP) [4]. It aims to streamline permits, scale financing and secure critical supply chains for net-zero technologies produced in Europe.

Spain operationalizes EU targets through its Plan Nacional Integrado de Energía y Clima (PNIEC). The July 2024 update tripled the country’s green-hydrogen ambition to 12 GW of electrolyzers by 2030 and requires 74 % of industrial hydrogen to be renewable by that date [6]. The plan also tightens the national 2030 emissions reduction target to –32 % versus 1990 and raises renewable-electricity targets (76 GW solar, 62 GW wind) [6].

These measures interact with continental carbon pricing: the reformed EU-ETS Phase IV will reduce the industrial emissions cap by 62 % from the 2005 baseline [10] and expand to maritime transport, while the Carbon Border Adjustment Mechanism (CBAM) progressively subjects imported ammonia and certain polymers to the same carbon cost as EU producers. Together, they create both regulatory pressure and market pull for decarbonized petrochemicals.

1.4 SPAIN’S PETROCHEMICAL SECTOR

Spain hosts the EU’s fourth-largest chemicals industry, contributing €82.5 billion in turnover (6 % of GDP) and 5.5 % of employment in 2023 [2]. Roughly 72 % of output was exported, making chemicals Spain’s second-largest export earner [2].

Three coastal clusters—Tarragona, Huelva/Algeciras and the Basque Country—house integrated steam crackers, refineries and fertilizer plants. Total industrial GHG emissions were 21 % of Spain’s total in 2023 [11], and petrochemicals are the single largest contributor within that share, around 60 Mt CO₂. Spain is a net exporter of refined products, shipping diesel, naphtha and kerosene across the Mediterranean and North-West Europe.

Decarbonization pilots are emerging: Repsol has secured €205 m in EU funding for a 2 Mt CO₂/yr offshore storage hub serving the Tarragona complex [12]. Regional initiatives such as the Basque Net-Zero Industrial Super-Cluster and Andalusia’s Green Hydrogen Valley illustrate growing sub-national momentum.

1.5 DECARBONIZATION PATHWAYS AND DEPLOYMENT GAP

Achieving climate neutrality in petrochemicals rests on four mutually reinforcing levers [7], [13]:

1. Shifting to low-carbon or circular feedstocks: By 2050 the NZE scenario requires more than one-third of global petrochemical inputs to come from recycled polymers, sustainable bio-naphtha or CO₂-derived intermediates rather than virgin oil and gas [13]. Today the share is in the single digits. Less than 10 % of the world’s plastic waste was mechanically recycled in 2023, with most of it landfilled or incinerated [7]. In Spain, the combined capacity of announced Spanish recycling and bio-feedstock ventures is still well under targets, as it is, it would still replace well under 2 % of the country’s present naphtha demand, an order-of-magnitude shortfall in relation to the NZE benchmark.
2. Electrifying high-temperature processes: A second wedge is to replace the fossil-fired furnaces of steam crackers—the heart of ethylene and propylene production—with electric heaters powered by renewables. The concept has cleared the pilot stage only this year: BASF, SABIC and Linde inaugurated a 6 MW electric furnace at Ludwigshafen in April 2024 that can cut cracker CO₂ emissions by 90 % [14]. Scaling such technology to hundreds of megawatts per cracker demands massive,

low-cost renewable electricity and grid reinforcement. Spain enjoys one of Europe's best solar-and-wind resource mixes, yet no Spanish chemical site has announced an electrified cracker program.

3. Replacing fossil-derived hydrogen with green or “blue” hydrogen: Petrochemicals already consume nearly one-fifth of global hydrogen, mostly produced from unabated natural gas. The IEA's NZE pathway raises low-emission hydrogen use in the sector to more than 110 Mt by 2050. Spain's updated Plan Nacional Integrado de Energía y Clima (PNIEC) therefore increased the domestic electrolyzer target to 12 GW by 2030.
4. Capturing the residual CO₂ that cannot be eliminated at source: Even with circular feedstocks and electrification, cracking and reforming processes leave an irreducible carbon stream that must be captured. The NZE map assigns around 190 Mt CO₂ yr⁻¹ of capture to the petrochemical sector worldwide by mid-century, but all industries together operated only about 50 Mt yr⁻¹ in 2025. Spain has started to close that gap: Repsol secured € 205 million in EU support for an offshore storage hub linked to the Tarragona cluster, sized for 2 Mt yr⁻¹ initially and expandable. At the regional level, the Basque Net-Zero Industrial Super-Cluster is coordinating shared CO₂ and hydrogen infrastructure among 23 industrial sites. Yet these ventures remain at the pre-FID (Final Investment Decision) or early construction stage.

1.6 MODELLING APPROACH AND OBJECTIVES

This thesis builds an open-source, Python / Pyomo optimization model that traces every ton of carbon, mass and energy through Spain's entire polymer value chain—from naphtha procurement and steam-cracking to the primary six bulk plastics production (PE, PP, PVC, PUR, PS, PET). The model minimizes the net-present system cost (2025 – 2050) while it honors external polymer-demand trajectories and explores the implementation of different decarbonization alternatives simultaneously.

What makes the framework distinctive is its process-level granularity: each primary unit (steam cracker, catalytic reformer, BTX loop, polymerization trains) is represented explicitly, characterized by its own process stoichiometry, energy consumption and carbon emissions.

At the same time, four mutually exclusive retrofit options—electric boilers, green-hydrogen furnaces, post-combustion CCS and a fully electric steam cracker—compete for deployment year by year. Capital builds, fixed O&M and legacy amortization are carried through vintage-specific cost streams, so the optimizer can weigh early-action retrofits against end-of-life replacement. All monetary flows (raw-material purchases, utilities, CAPEX annuities, fixed O&M, direct and indirect CO₂ charges) are discounted with a user-supplied real WACC.

The model delivers, for every year up to 2050, the cost-optimal capacity mix, throughput schedule and emissions profile of Spain's petrochemical sector, together with marginal abatement costs and technology-specific investment needs. Those outputs allow policymakers and industry stakeholders to benchmark feasible decarbonization pathways against national (PNIEC) and international (IEA, EU) climate targets, and to identify the levers—CCS, electrification or green hydrogen—that unlock the steepest emission cuts at the lowest system cost.

1.7 ALIGNMENT WITH SUSTAINABLE DEVELOPMENT GOALS



Figure 2 Project alignment with SDGs

This project also aims to align with the United Nations' standards of sustainable development goals, mainly although not exclusively, adhering to the following:

- **SDG 7: Affordable and Clean Energy** – The project explores pathways for integrating the reduction of fossil fuel dependency in the petrochemical sector, which aligns with the goal to increase the share of clean energy consumed.
- **SDG 9: Industry, Innovation, and Infrastructure** – The petrochemical industry is foundational for sustainable industrial development in Spain. This goal aligns seamlessly with the project’s scope of work.
- **SDG 12: Responsible Consumption and Production** – The research on integrating circular economy practices within the petrochemical sector directly addresses this goal. By assessing recycling, reuse, and waste reduction methods, the thesis promotes sustainable resource management, reduces environmental impact, and moves the sector towards a closed-loop production model.
- **SDG 13: Climate Action** – The project is rooted in the objective of mitigating climate change by assessing pathways to decarbonize the petrochemical industry in Spain. The research will support ongoing national and European efforts to achieve this goal.

Chapter 2. CONTEXT

Strategic energy planning models are essential tools for enabling informed decision-making in the energy transition [15]. Energy policymakers and corporations use linear or non-linear optimization models with long-term strategic planning goals, to assess the impact of different macro-economic scenarios and to show the most optimal behavior of the energy sector.

In the context of optimization models, this project will be developed from a bottom-up, partial equilibrium perspective. Bottom-up means that the model will calculate general outputs by aggregating low-level technically-detailed values. Partial equilibrium means that the model doesn't consider interactions between the fluctuation of the energetic variables and their effect on the economy.

*conceptual illustration of relations in models: partial equilibrium (top left), general equilibrium (top right) and integrated assessment models (bottom).
Source: own elaboration.*

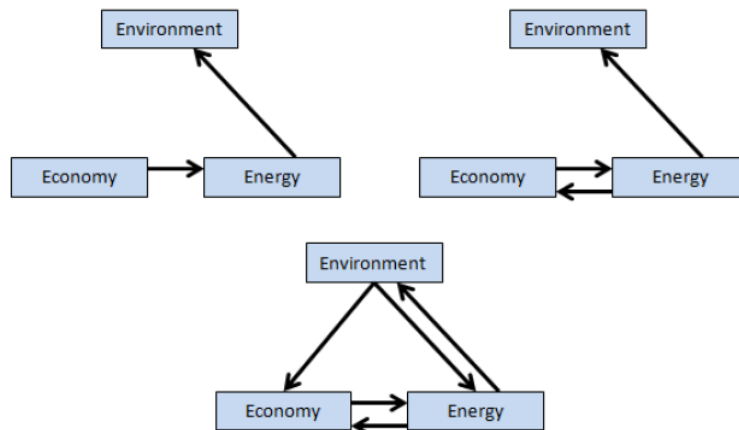


Figure 3 Types of energy planning models [2]

As illustrated in Figure 2, partial equilibrium models obtain energy demand from input data on economic activity, and they calculate how this demand will be met while being restricted by emissions costs as well as other traditional parameters. The main advantage of these types

of models in contrast to general equilibrium and integrated models is that they allow for higher technical precision when modelling [15].

2.1 THE MODELLING CHALLENGE

Energy-systems modelling has evolved from the engineering-style calculators built in the 1970s to today's integrated assessment frameworks that link technology, macro-economy and climate, parameters that enable these frameworks to drive decision making considering a more holistic view. López-Peña's state-of-the-art review organizes this landscape along three axes—economic closure (partial vs general equilibrium), technological depth (bottom-up vs top-down) and temporal representation (static vs dynamic)—and traces the lineage from PIES through EFOM and MARKAL to contemporary tools such as TIMES, POLES, EPPA and NEMS. Within these broad platforms, heavy industry is often compressed into a single “other industry” node; the petrochemical chain's intricate feedstock and by-product loops therefore remain hidden. Meeting mid-century climate goals exposes the limits of that aggregation and calls for dedicated, high-resolution linear-optimization models able to capture the sector's stoichiometric balances, retrofit choices and infrastructure constraints.

There are, of course, exceptions. The IEA's chemical-sector TIMES model tracks region-by-region capacity vintages and retrofit options for primary chemicals like high-value olefins and ammonia, but polymers are relegated to an aggregate “simulation module” with no optimization levers [16].

Academic work on petrochemical supply chains exists as well, typically single-site or short-horizon LP/MILP formulations aimed at weekly production planning or inventory control, e.g. the PuLP implementation for a C4 complex [17]. These models reach fine technical resolution but stop at the plant gate, lack forward vintaging and rarely publicize their data; open-source releases are even scarcer.

Petrochemical facilities run quasi-continuously, converting hydrocarbons into thousands of intermediate and final products. Decisions span:

- Discrete capacity choices (e.g. whether to retrofit a cracker with electric furnaces or install post-combustion CCS).
- Continuous operating variables (steam-cracking severity, recycle ratios, by-product disposition);
- Rigid stoichiometric and energy balances linking carbon, hydrogen, chlorine or nitrogen atoms across processes.

Capturing these features demands a modelling framework able to:

- Honor strict linear conservation rules.
- Accommodate thousands of technology–period combinations without exploding computationally.
- Deliver interpretable economic signals (marginal abatement costs, fuel–feedstock arbitrage values) for policy design.

Against that backdrop, this project intends to occupy an unfilled niche:

- Sector scope. It represents the entire polymer value chain—steam cracking, aromatics reforming, six finished plastics, related utilities—and embeds four mutually exclusive decarbonization levers (H₂ furnaces, CCS, E-boilers, E-crackers) at unit level.
- Temporal scope. A multi-period horizon (2025-2050) with endogenous retire-and-build decisions, discounting and vintage-specific CAPEX annuities.
- Open architecture. All parameters live in a human-readable Excel file; the code is pure Python/Pyomo under an open license, enabling peer review and local adaptation—something none of the proprietary refinery LPs or the IEA TIMES database presently offer.
- Circular-material hooks. Although still optional, the algebra already allows non-energy raw-material balances and future recycling loops, paving the way for circular-economy constraints that do not feature in existing petrochemical optimization studies.

In short, earlier work either aggregates petrochemicals away inside macro-energy models or solves highly specific planning problems without long-term decarbonization dynamics. This project bridges that gap by delivering a publicly documented, long-range, techno-economic linear program that retains the stoichiometric fidelity required to test deep-abatement pathways for polymers.

2.2 EXISTING PETROCHEMICAL OPTIMIZATION LITERATURE

The literature that applies linear or mixed-integer optimization to petrochemicals falls into three loosely connected strands, each with clear strengths but also with gaps that motivate the present model.

1. Sector modules embedded in energy-system frameworks.

The International Energy Agency's chemical-sector TIMES model solves a discounted linear program for thirty-nine world regions and underpins reports such as *The Future of Petrochemicals* [18]. It endogenizes technology choice for high-value chemicals (ethylene, propylene, BTX, ammonia, methanol) yet treats most polymers through an ex-post simulation loop, aggregated by region rather than by plant. No open data set is released, and unit-level material balances (steam, utilities, by-products) are coarsened into yield factors.

2. Plant and site-scale LP/MILP models for short-term scheduling.

Since the classic Exxon Mobil refinery LPs, dozens of papers optimize weekly production plans or supply-chain logistics for single complexes—e.g. Schulz et al.'s MINLP of a C₄ chain [19]. These formulations reach exquisite technical depth (heat curves, recycle loops, grade-segregated storage) but are myopic in time: they assume fixed capacities, ignore future decarbonization levers and rarely extend beyond one financial year.

3. Decarbonization studies focused on the steam cracker.

Recent work explores alternative furnace fuels (electricity, hydrogen) or post-combustion CCS using single-unit optimization or techno-economic life-cycle models—see Technip Energies’ roadmap and multi-objective LCA/optimization studies in the academic press [20]. While valuable for benchmarking specific retrofits, these one-process analyses cannot show how cracker choices ripple through a polymer line-up or a site-wide utility network.

What remains missing is an open, multi-period, bottom-up linear program that (a) spans the full polymer value chain, from naphtha procurement to PE/PP/PVC/PUR/PS/PET output, (b) couples four competing decarbonization levers (CCS, green-H₂ furnaces, electric boilers, e-cracker) within the same optimization, (c) carries vintage-specific CAPEX and OPEX over a 25-year horizon, and (d) preserves stoichiometric balances for carbon, hydrogen and chlorine so that indirect energy penalties and CO₂ liabilities are accurately priced. The model developed here is designed to close exactly that gap.

2.3 IDENTIFIED GAPS AND CONTRIBUTION OF THE PRESENT WORK

The survey above makes two things clear. First, high-level energy-system tools give a broad sense of where petrochemicals might head, yet they collapse the sector into a few archetypal reactions, suppressing the material loops, vintage effects and lever interactions that ultimately decide feasibility. Second, the detailed plant-LP literature delivers rich chemistry but is either short-horizon or proprietary and therefore unsuitable for policy exploration. Four concrete gaps emerge:

1. Multi-lever retrofit competition.

Existing bottom-up TIMES variants allow a single decarbonization choice per asset class (e.g. “ethylene-CCS”), whereas real complexes face competing options—post-combustion capture, E-boilers, green-H₂ furnaces or a brand-new E-cracker. This model instantiates four mutually exclusive levers per polymer family, lets them build or phase-in at different rates and prices them against one another every year.

2. Legacy-CAPEX bookkeeping.

Most long-range LP/MILP models treat the base year as sunk and cost-free; decisions start only when new capacity is added. Yet in capital-intensive industries, half the 2050 fleet is already on the books and still being amortized.

This project introduces a “three-vintage” legacy stream* that keeps the annuity of assets built 15, 10 and 5 years before the horizon start alive in the objective, so early-retirement penalties and stranded-asset risk are captured endogenously.

3. Utility–feedstock coupling with carbon pricing.

Cracker fuel, boiler steam and grid electricity interact under a single CO₂ price, but the IEA TIMES module and most site-LP papers pin these flows exogenously.

This formulation links fuel switches, CCS capture ratios and declining grid-EFs through a unified carbon account, paving the way for the dynamic arbitrage between electricity, natural gas and hydrogen.

4. Circularity and recycling.

Open-MASTER, EnergyScope and OSeMOSYS have begun adding recycling to final-energy demand, yet petrochemicals lack a stoichiometric industry specific description for raw materials. This project embeds optional commodity rows for recycled naphtha, pyrolysis oil and other oil derivatives, enabling future circularity constraints without rewriting the core algebra.

Bringing these elements together yields a public, fully documented optimization platform that sits between macro energy models and proprietary refinery LPs: detailed enough to trace atoms, long-term enough to test net-zero roadmaps, and transparent enough for replication and peer review. That combination—multi-lever retrofits,

vintage-aware costs, an integrated carbon-fuel-electricity balance and circular-material placeholders—constitutes the main contribution of the present work.

Chapter 3. PRODUCING PLASTICS

As is widely known, plastics are oil derived products than undergo chemical and physical transformations to become the final product. Oil and all of its adjacent industries consume c.120 Mb/d [21], of which petrochemical products account for c.25%, with share growth being forecasted until 2050, when they will represent c.40-50% of all consumption [21].

Currently, the petrochemical industry growth is mainly driven by the boost in consumption of plastics, textiles and other oil-based materials [21]. In Spain, the petrochemical industry is responsible for the contribution of c.6% of GDP [11], generating almost 800,000 jobs and being the second largest export industry for Spain's economy.

Plastics are one of the most relevant subsets of all petrochemical products due to their forecasted growth [21], acting as one of the key drivers of this industry in relation to the energy transition.

3.1 OIL & GAS PRODUCTS

The petrochemical value chain involves several consecutive processes that describe the flow of materials from extraction of crude oil to conversion to end products.

The petrochemical industry sits at the intersection between upstream energy supply and a large array of downstream manufacturing sectors. Although plastics are the focus of this thesis, a clear view of the entire value chain—from crude-oil extraction through to finished chemical products—is essential, both to map material flows and to identify leverage points for deep decarbonisation.

Crude oil enters a refinery as a complex hydrocarbon mixture. Atmospheric and vacuum distillation separate it into light gases (C₁-C₄), naphtha (C₅-C₁₁), kerosene, diesel and gasoil, and heavy residues [22]. Downstream conversion units (fluid catalytic cracking, hydrocracking, coking) break down the heavier and lower value fractions into lighter and

higher value ones, maximizing transport-fuel yields while generating valuable co-products—most notably liquefied petroleum gas (LPG), naphtha and light cycle oil, which become the principal feedstocks for petrochemicals [22]. Even inside a petrochemical complex, some material still ends its life as fuel: for instance, steam crackers bleed off heavy fuel oil and hydrogenated pyrolysis gasoline expressly “sold as fuel”. These fuels currently account for c. 60-70% of all oil consumption, but are expected to decrease to c.30-40% by 2050, in line with energy transition plans [21].

Group	Typical products	Main use
Fuels & energy carriers	LPG, gasoline, jet/kerosene, diesel, fuel oil, refinery gas	Mobility, heat & power
Petrochemical feedstocks	Ethane, propane, butanes, naphtha, condensate	Cracked to olefins & aromatics, then polymers
Fertilizer feedstocks	Natural-gas-rich synthesis gas	Ammonia to urea, ammonium nitrate, etc.
Specialties & others	Solvents, synthetic rubber, fibers, detergents, performance chemicals	Consumer & industrial goods

Table 1 Oil&Gas product categories and main uses [22]

In Table 1, the use cases of oil derived products have been classified into four categories—fuels & energy carriers, petrochemical feedstocks, fertilizer feedstocks and others—which exhaustively summarize the main use cases in the industry. For the purpose of this project, only the petrochemical feedstock category will be dealt with, as the detail needed to examine and accurately represent all categories would be excessive and not practical for the goal of this project.

3.2 PETROCHEMICAL PRODUCTS

The petrochemical value chain is characterized by several “building-block” molecules—the light olefins (ethylene, propylene, butadiene), the BTX aromatics (benzene, toluene, xylenes) and methanol—obtained from steam-crackers, refinery units or syngas routes [23]. These “building-block” molecules, as mentioned before, are a subset of all oil & gas derivatives, and will be the focus of this project.

Through successive and different conversion steps these intermediates fan out into several broad families of products, which can be summarized into four main categories:

- Nitrogenous fertilizers: ammonia synthesized from fossil-based syngas transformed to urea, ammonium nitrate, ammonium phosphate and other derivatives. Fertilizers are the single largest mass output of petrochemicals: in 2013 nitrogen fertilizers together with other thermoplastics already accounted for just over 60 % of all chemical products by weight, with ammonia alone absorbing 24 % of total feedstock [23]. It is also worth mentioning that these categories are not completely opaque as for example, ammonium nitrate is valued both as a high-nutrient fertilizer and as the oxidizer in most civil explosives.
- Plastics and synthetic rubbers: the diverse family of thermoplastics, thermosets and elastomers derived mainly from ethylene, propylene, styrene, vinyl-chloride or BTX aromatics. Thermoplastics dominate global polymer demand and, alongside fertilizers, are the other great mass flow in the petrochemical value chain [23]. These will be the focus of the project.
- Explosives and propellants: beyond ammonium nitrate, nitration of aromatics (e.g., toluene → TNT) or glycerin (nitroglycerin), this category links refinery-origin feedstocks to military and mining products; it also sits on the same backbone that feeds dyes for the paint and textile industries among others [23].
- Other large-volume derivatives: solvents (e.g. acetone), detergents, synthetic fibers (polyester, nylon), resins and adhesives, form the final category of products in the petrochemical value chain [23].

3.2.1 PLASTIC PRODUCTS

To further give context to the scope of this project, a simplistic view over the plastics production value chain has been elaborated.



Figure 4 From crude oil to plastic products (own elaboration)

As shown in Figure 4, in broad terms, the process from crude oil to plastic products (e.g. plastics bottles, scrubbing sponges), can be summarized in 4 steps.

First, the extracted crude oil is treated at a refinery, where crude oil is broken down into light and heavy fractions through distillation and other processes. The main products during this stage are monomers such as gasoline or natural gas, more specifically and in the interest of this project: naphtha, ethane, propane and butane. These compounds drive the production of the majority of plastics [23] and for that reason, they will be the main protagonists to characterize the industry appropriately. As a result of this conversion process, ethylene, propylene and other monomers are produced.

Next, the intermediate monomers are polymerized to form the final chemical compound that is used to produce the physical product. Following the example of ethylene, the polymer derived from this intermediate product is polyethylene. Normally, the products of this phase can be found in pellet form, which is useful for cheap transportation as it can be stored in low volumes when compared to the end products.

Finally, the polymers are conformed into their final shape through physical and chemical processes. Some examples of processes used to produce the end products are:

- Injection molding: melts pellet and injects the melt into a cooled mold to create complex, high-precision parts [23].

- Extrusion blow-molding: forms continuous tubes that are inflated in a mold to make bottles, films or hollow containers [23].

3.2.2 SCOPE OF THIS PROJECT

The European commission accounts for over 70,000 end products in its Large Volume Organic Chemicals Best Available Techniques report of 2017 [24]. For this reason, a very relevant task of this project has been to adequately capture the largest amount of information of the plastics value chain, without reaching unmanageable levels of products and processes.

Due to the nature of the project, several indicators could be used to perform an 80-20 rule to extrapolate the information of the top 80% of the information to the whole industry. Classifications by mass—as a percentage of total industry consumption—or energy were investigated, however, in the end, carbon emissions have been chosen as the better proxy to decide which compounds and products to include in the scope of the project.

Carbon emissions have been chosen due to the nature of the project—evaluating the decarbonization of the petrochemical industry—and have driven the selection of processes and products to be studied for the rest of the project.

Plastics family	Life-cycle emissions (Mt CO ₂ -eq)	Share of plastics emissions
Polypropylene (PP)	228	16%
Polyurethane (PUR)	164	12%
PE (L/LLDPE)	196	14%
High-density PE (HDPE)	159	11%
Polyethylene terephthalate (PET)	137	10%

Polystyrene (PS)	119	8%
Polyvinyl chloride (PVC)	102	7%
Subtotal (7 resins)	1,105	79%

Table 2 Plastics emissions [25]

Table 2 has been elaborated to summarize the plastics life cycle emissions and to provide an indicator of how accurately the industry is being represented with these compounds with the goal of deriving a linear optimization model from the description of the processes associated to the production of these compounds.

According to [25] and to Table 2, with these seven compounds the industry is represented at an 79%, which has been deemed and appropriate trade-off between complexity and accuracy, and for this reason, these will be the compounds studied in the following chapters.

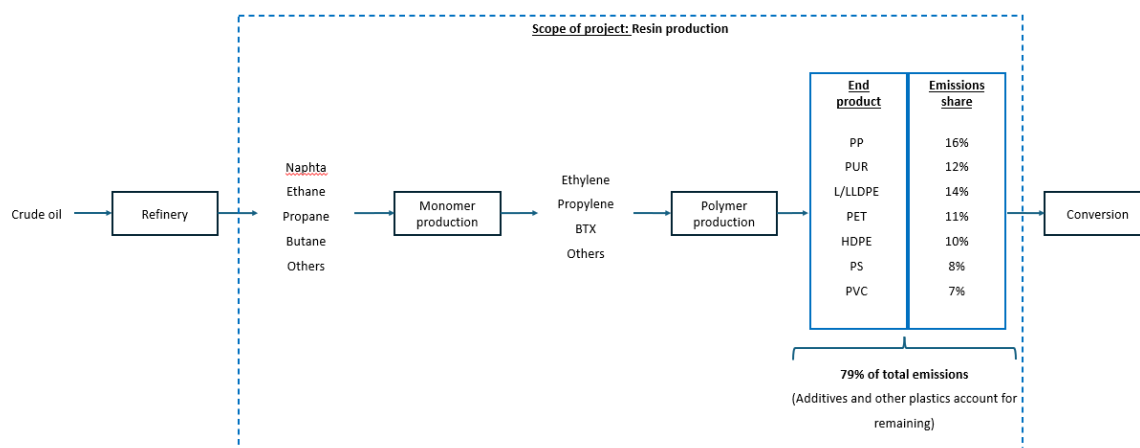


Figure 5 Plastics included in the scope of this project (own elaboration)

Figure 5 has been elaborated to illustrate conceptually the scope of the project in terms of steps of the value chain that will be included. As previously discussed, there are over 70,000 end products characterized and for that reason, including the final conversion step of the

value chain, which only includes the physical transformation of the pellets to final products has been left out of the scope.

Upwards of the value chain, the refinery step of the process has been decided not to be included, as the goal of the project is to characterize the plastics industry, rendering oil and gas inputs out of the scope.

3.3 METHODOLOGY FOR DESCRIPTION OF PRODUCTION PROCESSES

To adequately represent any process of the plastics value chain—from input feeds to final products—a general approach that captures all relevant parameters in any process has been defined, then the specific parameters which are relevant for the model have been deducted, and finally, these parameters have been searched for in every process (e.g. PET production) that is relevant for this project. This approach has been defined as it provides several key advantages for the execution of the project, which are mainly:

- First, it guarantees consistency: every process is described with the same structural logic, so mass, energy and emissions data can be compared or summed without hidden misalignments.
- Second, the framework is scalable and extensible: once the “master set” of parameters exists, adding a new plastic or a future recycling pathway is little more than filling in the relevant rows, not redesigning the model.

It could be argued that the project could have used theoretical chemical and energy balances to determine the energy consumption and emissions derived from the production of any plastic. However, this study remains out of the scope of the project, as it would entail describing and analysis of all relevant sub-processes at a site level, and that work would yield little to no value when compared to studying processes as “black boxes”.

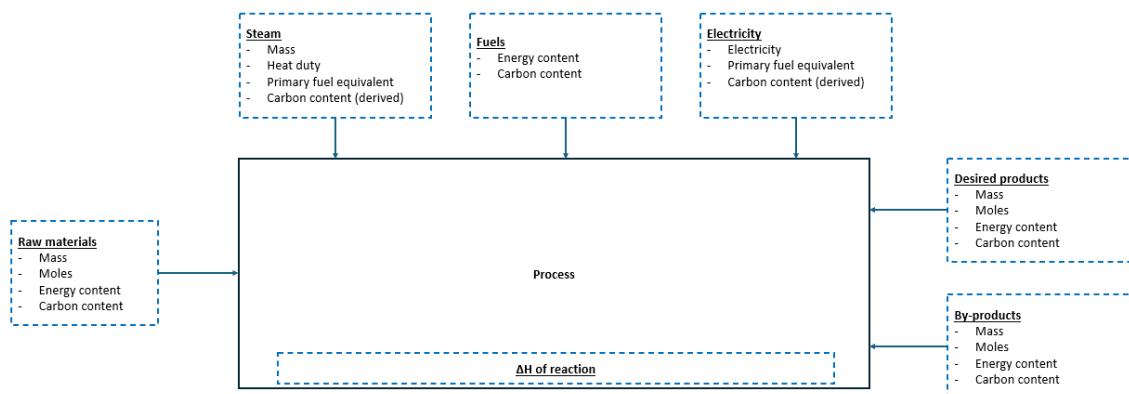


Figure 6 Process balance (adapted from [26])

The scheme shown in Figure 6, has been elaborated to capture the general scope of any process, treating it as a “black box” and only focusing in inputs and outputs.

To understand each of the categories described in Figure 6, the following description has been elaborated [26]:

- Mass variables: For every inlet or outlet of each process, a stream can be defined in moles so that through stoichiometry, its mass properties can be characterized. Chemically, this is the unequivocal way of describing any process. However, as previously expressed, for the scope of this project, all of the mass related variables are not relevant, and so, only mass input to output ratios will be considered, leaving stoichiometry aside. The chemical reactions of the processes will be defined, but these will not be used to characterize the input to output ratios but rather existing literature that is based on real steam crackers.
- Energy variables: Three key variables—steam, fuel and electricity—have been identified as exhaustive for the description of the energy flows in any process. It must be mentioned, that these streams represent the actual consumption of the processes, but that due to the nature of the reactions occurring in each—exothermic or endothermic—the total energy balance for the processes can be very different to the characterization provided in this project.

- Steam provides the indirect heat that reactors, distillation columns, and pellet dryers among other equipment need, via coils, jackets or reboilers at controlled pressures [27]. It is normally logged as a mass flow, but the key thermodynamic number is its heat duty, defined as the enthalpy difference between the supply conditions (e.g. 10 bar/280 °C for medium-pressure steam) and returned condensate. As this project doesn't need to characterize the whole process, but only the relevant variables of each, to link this duty to primary resources, this project considers a division by a nominal 90 % boiler efficiency [26] and records a primary-fuel equivalent plus the associated CO₂ from that boiler fuel, which will be key variables extracted.
- Fuel supplies the direct high-temperature heat for cracking furnaces, heater banks, incinerators and flare systems, often by burning process off-gas or natural gas [27]. It will be used in the model directly with its lower heating value in any process, and emissions associated to the fuel will also be taken into account.
- Electricity drives all rotating and electromechanical loads [27]—compressors for ethylene refrigeration, polymer-melt extruders, pumps, agitators and the automation network that steers them. Because every duty is ultimately a kWh draw, this stream is needed to capture the full spectrum of applications that might substitute for steam or fuel. A fixed power-station efficiency is used in the project (41 % [26]) to convert that electricity to a primary-fuel demand, and the corresponding carbon content is attached based on the grid's fuel mix, which will allow for the model to include the decarbonization of the grid as a lever for the industry decarbonization.
- Emissions variables:
 - Process-intrinsic carbon belongs to the molecules that each process chemically makes or breaks. By comparing the carbon content of feeds, products and by-products, it is possible to isolate the fraction of feed carbon that is oxidized to CO₂. In this project, these emissions will be described as “carbon losses, reaction”.

- Utility-related carbon arises when external fuels are burned to raise steam or electricity. These emissions are counted separately and will be described as “carbon losses, energy use” for the rest of the project.

3.4 MONOMER PRODUCTION

As a first step of the scope of this project, and as previously described, the initial phase of the plastics value chain receives inputs from oil refineries and transforms these inputs into monomers through various chemical processes.

3.4.1 STEAM CRACKING

Steam cracking is a petrochemical process in which light or mid-range hydrocarbons—natural-gas liquids such as ethane, propane and butane, plus petroleum naphtha or gas-oil—are mixed with steam and rapidly heated in tubular furnaces. At the high furnace temperature, the molecules “crack,” yielding a slate rich in olefins (mainly ethylene and propylene), aromatics (e.g., benzene) and hydrogen gas [28].

Steam cracking generates olefins, it is the primary industrial route to ethylene—regarded as “the backbone of the chemical and plastics industry” because it is later polymerized into polyethylene and many other materials [28]. It also co-produces hydrogen, the cracking reactions liberate significant hydrogen, which plants typically burn in the furnace tail-gas for heat, but which can also be recovered as a marketable low-carbon H₂ stream.

Related to hydrogen usage, two main typologies of steam crackers can be characterized:

1. Hydrogen as an internal fuel (group A): the H₂ liberated during the process, carries about 1.6 GJ. Together with the methane they cover roughly four-fifths of the 10 GJ t⁻¹ heat duty, and therefore, only c.2 GJ t⁻¹ of external natural gas is then needed for steady operation [28]. Because the hydrogen fraction is carbon-free, burning it lowers the CO₂ intensity of the overall process.

2. Hydrogen as an exportable co-product (group B): some crackers instead treat the tail-gas in a pressure-swing-adsorption (PSA) unit, recover 99.9 % pure H₂, compress it and send it to pipeline [28]. Removing the H₂ heat leaves a gap in the energy demand, which is generally covered by using natural gas, therefore increasing the carbon intensity of the process.

3.4.1.1 Mass balance

Steam cracking can be executed with a variety of feed compositions, depending on the production facility targets, feedstocks will be heavier on certain compounds (e.g. ethane) when the target is to maximize production of a certain output.

Input	Ethane	Propane	n-Butane	Naphtha	Gas-oil
Output					
H ₂	0.062	0.019	0.014	0.011	0.009
CH ₄	0.058	0.26	0.22	0.14	0.11
C ₂ H ₄ (ethylene)	0.80	0.44	0.41	0.30	0.28
C ₃ H ₆ (propylene)	0.019	0.17	0.19	0.17	0.14
Butadiene (C ₄ H ₆)	0.028	0.033	0.044	0.048	0.058
Benzene (C ₆ H ₆)	0.0086	0.024	0.030	0.064	0.055
Other liquids (P-gasoline, BTX, fuel-oil, etc.) ~ 0.06–0.18 kg depending on feed					

Table 3 Steam cracking mass yields (%) [28]

Table 3 shows the proportion of input to output mass ratios based on the type of input introduced into the steam cracker. This table is of great use to understand the nature of the steam cracking process, as it displays perfectly the variety of output compositions based on the input stream.

However, this table is not enough to characterize the steam cracking process, because the question arises, what should the specific input ratio to be used in the model be? To answer this question, the average blend of all U.S. crackers in 2016 has been used [28].

Flow	Group A	Share A	Group B
Ethylene	503 kg	50.3 %	503 kg
Propylene	116 kg	11.6 %	116 kg
Pyrolysis gasoline (aromatics)	49 kg	4.9 %	49 kg
Butadiene	38 kg	3.8 %	38 kg
Hydrogen (tail-gas basis)	17 kg	1.7 %	-
Methane (tail-gas basis)	17 kg	1.7 %	17 kg
Other C ₄ / C ₅ , BTX, fuel-oil	117 kg	11.7 %	117 kg
Total saleable + fuel gas	857 kg		840 kg
Non-condensables & losses	c.1 %		c.1 %

Table 4 Steam cracking output per ton of input [28]

Table 4 shows that ethylene is the main product of the steam cracking process, accounting for c.50% of all the products (by mass). For this project, BTX—Benzene, Toluene and Xylene compounds—are also relevant, and pyrolysis gasoline is primarily composed of those three compounds, so, for modelling purposes, Table 5 shows the BTX ratios included in the model.

Species	wt % of raw pygas	Mass in 49 kg pygas stream

Benzene	18 – 25 % (mid-case 21 %)	c.10 kg
Toluene	19 – 23 % (mid-case 22 %)	c.11 kg
Xylenes	24 – 28 % (mid-case 27 %)	c. 13 kg
C ₉ ⁺ aromatics & saturated C ₅ –C ₉	balance ($\approx$ 30 %)	c.15 kg
Total	100 %	49 kg

Table 5 Pygas BTX ratios

Feedstock	Share of total feed mass
Ethane	34.9 %
Propane	18.5 %
n-Butane	4.5 %
Naphtha	41.5 %

Table 6 Steam cracker input average composition [28]

Table 6 shows the industry average—for 2016 U.S. crackers—of input composition, it must be noted that the total composition adds up to 99.4% as other minor compounds that are not relevant for the scope of the project account for the remaining 0.6%. This average composition is the one that provides the outputs shown in Table 4.

3.4.1.2 Energy balance

Utility stream	Group A	Group B
Furnace heat supplied by:		
Hydrogen in tail-gas	1.61 GJ / t of feed	–
Methane in tail-gas	6.07 GJ / t of feed	6.07 GJ / t of feed
C ₂ – C ₄ fragments	0.24 GJ / t of feed	0.24 GJ / t of feed
Purchased natural gas	2.06 GJ / t of feed	3.67 GJ / t of feed
Subtotal furnace fuel	9.98 GJ / t of feed	9.98 GJ / t of feed
Electricity	~ 0.02 GJ / t of feed (negligible)	~ 0.02 GJ / t of feed (negligible)
Electricity for PSA and H ₂ compression	–	0.031 GJ / t of feed (negligible)
Total external energy purchased	2.06 GJ / t of feed	3.67 GJ / t of feed

Table 7 Steam cracking energy consumption [28]

Table 7 shows the energy consumption of the steam crackers in the U.S. in 2016, divided into groups A and B as previously mentioned. The total furnace fuel consumption (9.98 GJ) is the same for both groups, however the difference lies in the total external energy purchased that is used for the furnace fuel. Since hydrogen fuel is exported in group B steam crackers, 1.61 GJ of ‘extra’ energy must be purchased for these group of crackers.

3.4.1.3 Emissions balance

To characterize the emissions derived from steam cracking, this project has performed research on several steam cracker life cycle analysis which cover the scope of this project and avoid going into detailed steam cracker processes description and characterization.

	kg CO ₂ -eq kg ⁻¹	Comments
Group A	1.05	Tail-gas H ₂ provides 16 % of furnace heat with zero carbon, so purchased fossil fuel is only 2.06 GJ
Group B	1.30	Losing the 1.61 GJ of zero-carbon H ₂ heat forces an extra 1.61 GJ of natural-gas firing

Table 8 Steam cracking emissions [28]

As seen in Table 8, emissions are higher for the Group B (hydrogen as co-product) by 0.25 kg / kg of feed due to the benefits of using hydrogen as a fuel for emissions reduction.

3.4.2 CATALYTIC REFORMING

Catalytic reforming is the step of the value chain that “redesigns the hydrocarbon molecules of the naphtha feed and performs aromatization”, turning a low-octane straight-run naphtha into a high-octane liquid called reformat while co-producing large amounts of hydrogen and some light gases [29]. Through this process, three main results are obtained [29]:

- Octane upgrade for fuels: reformat typically pushes the research-octane number (RON) from < 70 in the feed to > 95, making it essential as a blending stock for gasoline.
- Feedstock for aromatics chemistry: the same aromatization reactions generate a BTX stream (benzene, toluene, xylenes) embedded in the reformat, which can be recovered and routed to the petrochemical chain.

- On-site hydrogen supply: each ton of naphtha yields about 10–15 kg of H₂, offsetting the need for dedicated steam-methane reforming elsewhere in the refinery and giving the unit a net negative GHG footprint when that credit is considered.

3.4.2.1 Mass balance

Catalytic reforming is similar to steam cracking in the way that a very heterogeneous feed stream is transformed into higher value discrete hydrocarbons that are used as precursors for the petrochemical industry or fuels for transport.

Category	Component(s) included	Wt % of naphtha
Aromatics – BTX	Benzene	1.45
	Toluene	4.06
	p-Xylene	0.92
	m-Xylene	2.75
	o-Xylene	0.87
Other aromatics	Ethylbenzene + C9+ others	3.83
Total aromatics		13.88
Olefins (all)		0.11
Paraffins	C3–C5 (propane → n-pentane)	17.31
	C6 (iso- & n-hexane)	11.30
	C7 (iso- & n-heptane)	9.20
	C8 (iso- & n-octane)	7.67

	C9 + (C9-C11 paraffins)	9.87
Total paraffins		55.35
Naphthenes	Cyclo-alkanes C5-C11	30.70

Table 9 Catalytic reforming naphtha composition [30]

Table 9 shows the composition by weight of the input naphtha stream into the catalytic reforming process. Most notably, BTX compounds account for 13.88% of the input stream by weight. These compounds will be the most relevant for the due to their use in later stages of polymer production in the plastics value chain. Several other key products of catalytic reforming such as paraffins and naphthenes are not relevant for the scope of this project as they are not key inputs to plastics production processes.

Stream	kg t ⁻¹ feed	% weight	Source
Reformate (total)	918		[29]
Benzene	34.1	3.72 %	[30]
Toluene	128.2	13.97 %	[30]
Xylenes (p + m + o)	144.0	15.69 %	[30]
Ethyl-benzene	28.7	3.13 %	[30]
C ₉ and other aromatics	331.0	36.05 %	[30]
Other paraffins + naphthenes + olefins	252.0		[30]
Hydrogen (export)	69.6		[29]

LPG (C ₃ - C ₄ mix)	10.4		[29]
Fuel-gas (C ₁ / C ₂)	1.7		[29]
Total products	1 000 kg		

Table 10 Catalytic reforming mass balance

Table 10 shows the output stream composition by weight. 91.8% of the total stream by mass is composed of the reformat hydrocarbons, among which benzene, toluene, xylene and ethyl benzene are used as precursors for producing some of the most widely used plastics (e.g. PUR, PVC).

C₉ stream (widely used for gasoline blending [30]), is the other primary output of the catalytic reforming process. As previously mentioned, one of the goals of this process is to produce higher octane and therefore higher valued hydrocarbons that are used in transportation.

3.4.2.2 Energy balance

Due to the production of hydrogen from the catalytic reforming process, it is considered to be a net energy producer, as hydrogen exports account for more energy than the process itself consumes [30].

Utility	GJ t ⁻¹ feed
Fired-heater duty (natural-gas fuel)	1.46
Electricity (compressors, pumps)	0.24
H ₂ exports	-8.35
Net purchased energy	-6.65

Table 11 Catalytic reforming energy balance [29]

To elaborate Table 11, the energy consumption provided by [29] has been divided by the feed flow (eg. $24.57 \text{ MW} / 60,605 \text{ t h}^{-1} = 1.46 \text{ GJ t}^{-1}$) and the resulting values for energy consumption are as shown. For hydrogen, the total output stream (69.6 kg) has been multiplied by its lower heating value of 120 MJ kg^{-1} to obtain the result shown.

3.4.2.3 Emissions balance

As catalytic reforming has been seen as a net energy exporting process, it is also a net negative process in terms of carbon emissions. However, this project has included emissions figures related to the H_2 exports but also related to the process emissions, so later on in the model it can be decided which scope to keep as part of the catalytic reforming process.

Contribution	g CO ₂ -eq kg ⁻¹ reformat	Calculation method
Process emissions	+123.1	[29]
Fired-heater fuel	113.1 (~ 91.9 %)	Figure 4 [29] shows heat duty is 91.9 % of the climate-change load; $0.919 * 123.1$
Electricity	9.0 (~ 7.3 %)	Figure 4: $7.3 \% * 123.1$
Catalyst regen.	1.0 (~ 0.8 %)	Figure 4: $0.8 \% * 123.1$
Hydrogen credit	-868.6	Difference between the substitution result (-745.5 g) and the gross 123.1 g
Net GHG	-745.5	[29]

Table 12 Catalytic reforming emissions

Table 12 summarizes the total emissions and creates a subdivision in electricity usage related emissions, fuel for process related work and hydrogen credit from the export of the H_2 produced.

3.5 POLYMER PRODUCTION

After transforming the refinery outputs to monomers, the process diverts to other facilities—even though many combine upstream and downstream production—with the task of transforming the monomers to the final chemical product that can be extruded or formed into the final products. This step of the process is the polymer production, and in this section, 6 key industry processes are developed to later include in the model. As previously described, these processes have been chosen as a good representation of the industry due to the elevated share of total emissions that they represent.

It is relevant to note that throughout this chapter, in the energy and emissions related figures, there will be two tables included. The first one will define the energy consumption unadjusted, which means that every point of data will represent the GJ of energy consumed per ton of product produced (i.e. oxidation from ethylene to produce ethylene oxide will be noted with the amount of energy used to produce 1 ton of ethylene oxide). Subsequently, an adjustment of these quantities will be made according to the mass balance performed for each process, meaning that each of the consumption flows will be scaled to the actual process consumption through the mass balances.

3.5.1 PET PRODUCTION

Polyethylene Terephthalate (PET) is produced from p-Xylene and Ethylene following several steps—oxidation, hydration and finally polycondensation—until the final molecule is produced. Although there are variants to this process, the specific variation has been chosen due to it being the principal PET production method [31].

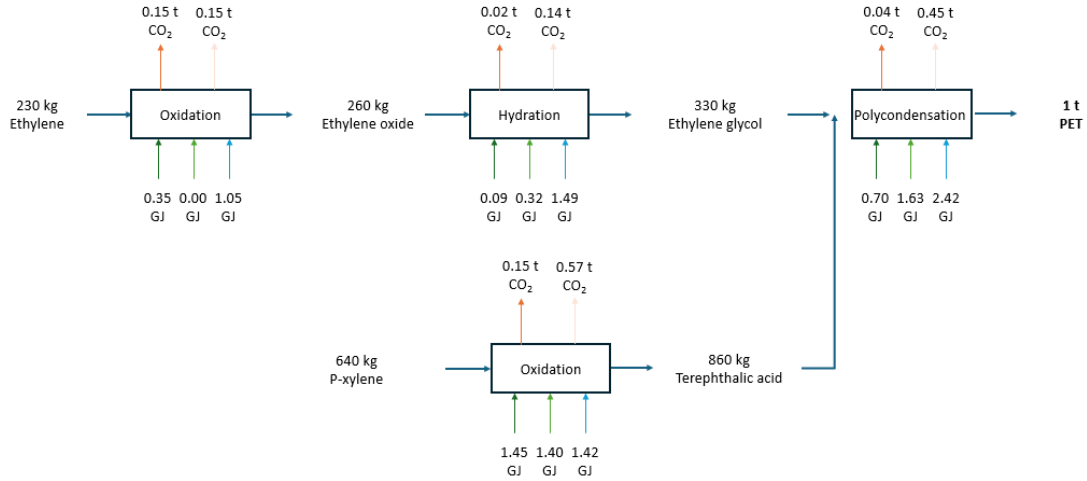


Figure 7 PET production process (own elaboration, [26])

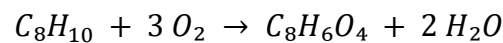
Figure 7 shows a schematic view of the production process of 1 ton of PET. Its main inputs—p-xylene and ethylene—are derived from processes in the previous step of the plastics production value chain.

3.5.1.1 Mass balance

The path from monomers to the final PET polymer can be summarized by the following steps:

1. p-Xylene → Purified Terephthalic Acid (PTA)

- Global reaction [32]:

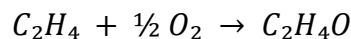


- p-Xylene (C₈H₁₀) is oxidized (using air/oxygen and catalysts) to form terephthalic acid (TPA).
- After hydrogenation (purification), PTA (C₈H₆O₄) is obtained.
- The minimum stoichiometric quantity needed to produce 1 t of PTA: 0.64 t p-xylene → 1 t PTA (using molar weights of 106.16 → 166.13 g mol⁻¹)

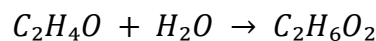
- A common rule of thumb is that about 0.66 ton of p-xylene is needed to produce 1 ton of PTA due to efficiencies of the process [32].

2. Ethylene → Ethylene Oxide (EO) → Ethylene Glycol (EG)

- Reaction from Ethylene - Ethylene Oxide [33]:



- Ethylene (C_2H_4) is partially oxidized to ethylene oxide (EO).
- EO is then hydrated to ethylene glycol (EG, $C_2H_6O_2$) [33]:



- Modern plants aimed at EG production can achieve nearly a 1:1 mass ratio of EO to EG, though some by-product di- and tri-ethylene glycol also form [34].
- Typically, c.0.65-0.70 ton of ethylene is required to produce 1 ton of EO, which then yields 1 ton of EG [34].

3. PTA + EG → PET

- PTA and EG undergo polycondensation in two main stages [31]:
 1. Esterification (or Transesterification) to form bis(hydroxyethyl) terephthalate (BHET).
 2. Polycondensation (under reduced pressure and elevated temperature) to form PET.
- In a typical PET process, about 0.86 ton of PTA and 0.34 ton of EG make 1 ton of PET [31].

4. Using all the numbers above to compute the final input to output ratios:

- p-Xylene needed: c.0.57 ton (to make c.0.86 ton PTA)
- Ethylene needed: c.0.24 ton (to make c.0.34 ton EG)
- PTA + EG: 0.86 t PTA + 0.34 t EG → 1.00 t PET

3.5.1.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Oxidation ($C_2H_4 \rightarrow$ ethylene-oxide)	1.02	0.00	3.09
Hydration (EO → ethylene-glycol)	0.26	0.94	4.37
Oxidation (p-xylene → TPA)	1.69	1.63	1.65
Polycondensation (TPA + EG → PET)	0.70	1.63	2.42

Table 13 PET production energy consumption (unadjusted for mass balance) [26]

Table 13 shows the unadjusted energy consumption of all the PET production sub-processes. This means that for each step, the total energy consumption has been characterized per 1 ton of feed.

Sub-process	Electricity (GJ / t of PET)	Fuel (GJ / t of PET)	Steam (GJ / t of PET)
Oxidation ($C_2H_4 \rightarrow$ ethylene-oxide)	0.35	0.00	1.05
Hydration (EO $\rightarrow$ ethylene-glycol)	0.09	0.32	1.49
Oxidation (p-xylene $\rightarrow$ TPA)	1.45	1.40	1.42
Polycondensation (TPA + EG $\rightarrow$ PET)	0.70	1.63	2.42

Table 14 PET production energy consumption (adjusting for mass balance)

Table 14 shows the adjusted energy consumption of all the PET production sub-processes scaled by using the previously described mass balances. This means that for each step, the total energy consumption has been characterized by the actual amount of mass used from each feedstock.

3.5.1.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ / t of PET]	CO ₂ (energy use) [t CO ₂ / t of PET]
Oxidation ($C_2H_4 \rightarrow$ EO)	0.45	0.43
Hydration (EO $\rightarrow$ EG)	0.05	0.41
Oxidation (p-xylene $\rightarrow$ TPA)	0.15	0.57
Polycondensation (TPA + EG $\rightarrow$ PET)	0.04	0.45

Table 15 PET production carbon emissions (unadjusted) [26]

Table 15 shows the unadjusted emissions of all the PET production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PET]	CO ₂ (energy use) [t CO ₂ /t of PET]
Oxidation (C ₂ H ₄ → EO)	0.15	0.15
Hydration (EO → EG)	0.02	0.14
Oxidation (p-xylene → TPA)	0.15	0.57
Polycondensation (TPA + EG → PET)	0.04	0.45

Table 16 PET production emissions (adjusted for mass balance)

Table 16 shows the adjusted emissions of all the PET production sub-processes scaled by using the previously described mass balances.

3.5.2 PVC PRODUCTION

Polyvinyl Chloride (PVC) is produced from Ethylene following a simplified 3 step process.

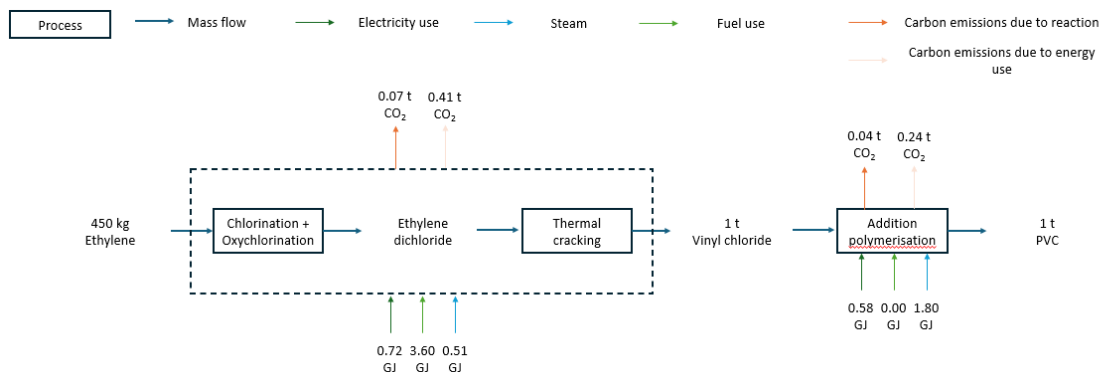


Figure 8 PVC production process (own elaboration)

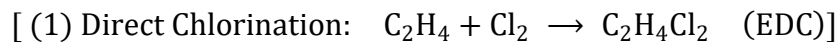
Figure 8 summarizes this process schematically, including mass input to output ratios, energy consumption and emissions associated with the process.

3.5.2.1 Mass balance

The process steps are as follows:

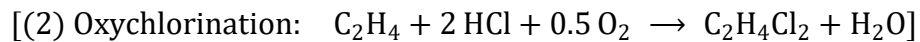
1. Vinyl Chloride Monomer (VCM) production

a. Direct chlorination [35]



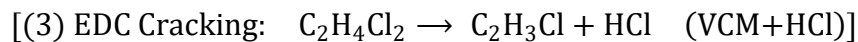
b. Oxychlorination [35]

- Combines HCl (by-product) with ethylene and oxygen to form more EDC (ethylene dichloride).



c. Thermal cracking of EDC [35]

- Vinyl chloride (VCM) is separated, while HCl is recycled to oxychlorination.



2. PVC polymerization

- Vinyl chloride monomer (VCM) undergoes addition (chain-growth) polymerization.
- Common methods: suspension, emulsion, or bulk polymerization [36].

3. Overall approximate mass balance (per 1 ton of PVC) [37]:

- Ethylene: c.450 kg
- Chlorine: c.760 kg
- Oxygen (for oxychlorination): c.85 kg
- Polymerization aids, initiators: a few kilograms, negligible

3.5.2.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Oxychlorination + thermal cracking to vinyl-chloride monomer	0.72	3.60	0.51
Addition polymerisation of vinyl chloride to PVC	0.58	0.00	1.80

Table 17 PVC production energy consumption (unadjusted) [26]

Table 17 shows the unadjusted energy consumption of all the PVC production sub-processes.

Sub-process	Electricity (GJ / t of PVC)	Fuel (GJ / t of PVC)	Steam (GJ / t of PVC)
VCM production (oxychlorination + thermal cracking)	0.72	3.60	0.51
Addition polymerisation (VCM → PVC)	0.58	0.00	1.80

Table 18 PVC production energy consumption (adjusted for mass balance)

Table 18 shows the adjusted energy consumption of all the PET production sub-processes scaled by using the previously described mass balances.

3.5.2.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ /t of intermediate products]	CO ₂ (energy use) [t CO ₂ /t of intermediate products]
Oxy-chlorination + thermal cracking (ethylene → VCM)	0.07	0.41
Addition polymerisation of VCM → PVC	0.04	0.24

Table 19 PVC production emissions (unadjusted) [26]

Table 19 shows the unadjusted emissions of all the PVC production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PVC]	CO ₂ (energy use) [t CO ₂ /t of PVC]
VCM production	0.07	0.41
Addition polymerisation	0.04	0.24

Table 20 PVC production emissions (adjusted for mass balance)

Table 20 shows the adjusted emissions of all the PVC production sub-processes scaled by using the previously described mass balances.

3.5.3 PUR PRODUCTION

Polyurethane (PUR) is produced from Toluene via a simplified 3-step process.

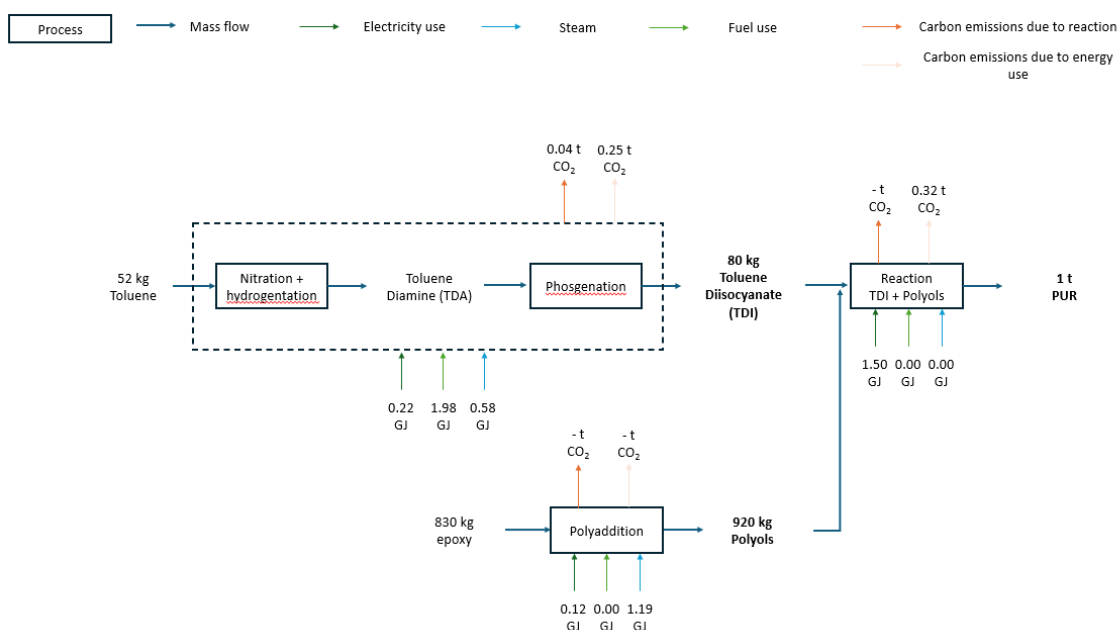


Figure 9 PUR production process (own elaboration)

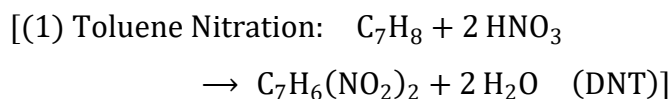
Figure 9 summarizes this process schematically, including mass input to output ratios, energy consumption and emissions associated with the process. It must be noted, that this is the PUR production process from toluene via the Toluene Diisocyanate (TDI) route, and there are other variants which have not been included in this description due to the sufficient nature of this variant as representative of all the variants.

3.5.3.1 Mass balance

1. Toluene nitration

Toluene (C₇H₈) is treated with nitric acid (plus sulfuric acid) to form dinitro toluene (DNT).

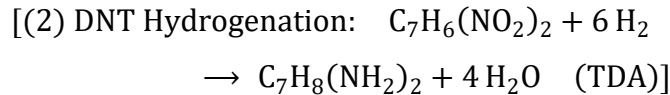
- Simplified reaction [38]:



2. DNT hydrogenation

Dinitro toluene (DNT) is hydrogenated (with H₂ over a catalyst) to produce toluene diamine (TDA).

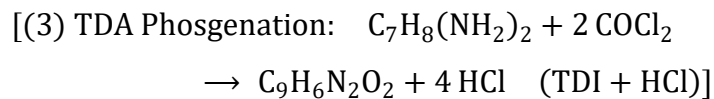
- Simplified reaction [38]:



3. TDA phosgenation

Toluene diamine (TDA) reacts with phosgene (COCl₂) to form toluene diisocyanate (TDI).

- Simplified reaction:



4. Polyurethane formation (TDI + Polyol)

TDI reacts with a polyol (e.g., a di- or tri-functional alcohol) to form polyurethane.

- General scheme [38]:



Typical mass balance:

- To make 1 ton of PUR [38]:
 - c.80 kg of TDI
 - c.920 kg of polyol
- TDI itself originates from c.52 kg of toluene (plus nitric acid, hydrogen, phosgene, etc.) once process yields are accounted for.

3.5.3.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Nitration + hydrogenation + phosgenation (toluene → TDI) — <i>aggregated</i>	2.76	24.76	7.25
Poly-addition (epoxy → polyols)	0.13	0.00	1.29
Final reaction (TDI + polyols → PUR)	1.50	0.00	0.00

Table 21 PUR production energy consumption (unadjusted) [26]

Table 21 shows the unadjusted energy consumption of all the PUR production sub-processes.

Sub-process	Electricity (GJ / t of PUR)	Fuel (GJ / t of PUR)	Steam (GJ / t of PUR)
TDI block (nitration + hydrogenation + phosgenation)	0.22	1.98	0.58
Poly-addition (epoxy → polyols)	0.12	0.00	1.19
Final reaction (TDI + polyols → PUR)	1.50	0.00	0.00

Table 22 PUR production energy consumption (adjusted for mass balance)

Table 22 shows the adjusted energy consumption of all the PUR production sub-processes scaled by using the previously described mass balances.

3.5.3.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ /t of intermediate products]	CO ₂ (energy use) [t CO ₂ /t of intermediate products]
Nitration + hydrogenation + phosgenation (toluene → TDI)	0.44	3.06
Poly-addition (epoxy → polyols)	0.00	0.00
Final reaction (TDI + polyols → PUR)	0.00	0.32

Table 23 PUR production emissions (unadjusted) [26]

Table 23 shows the unadjusted emissions of all the PUR production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PUR]	CO ₂ (energy use) [t CO ₂ /t of PUR]
TDI block	0.04	0.25
Poly-addition (polyols)	0.00	0.00
Final reaction (PUR synthesis)	0.00	0.32

Table 24 PUR production emissions (adjusted for mass balance)

Table 24 shows the adjusted emissions of all the PUR production sub-processes scaled by using the previously described mass balances.

3.5.4 PS PRODUCTION

Polystyrene (PS) is produced from Benzene and Ethylene.

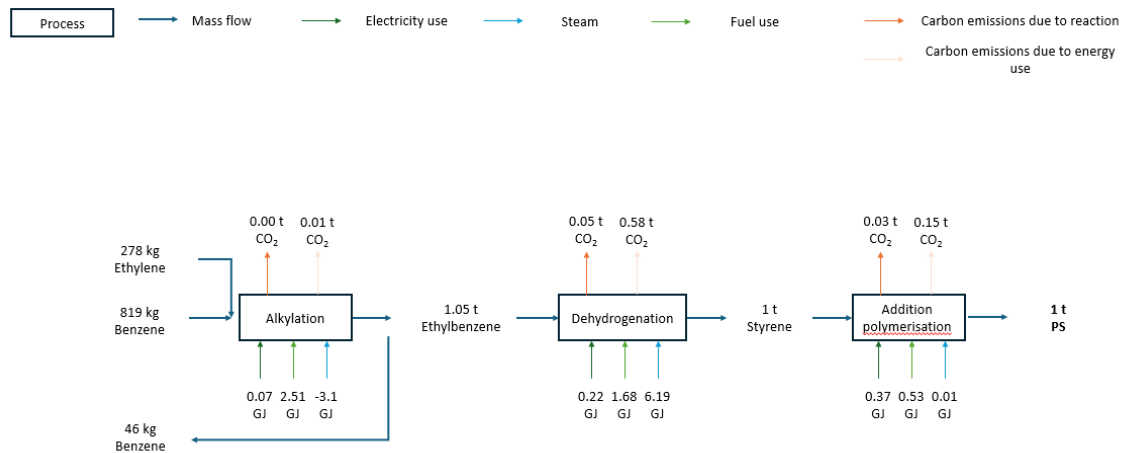


Figure 10 PS production process (own elaboration)

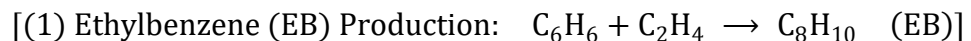
Figure 10 summarizes this process schematically, including mass input to output ratios, energy consumption and emissions associated with the process.

3.5.4.1 Mass balance

1. Ethylbenzene (EB) production

Alkylation of benzene (C₆H₆) with ethylene (C₂H₄) to form ethylbenzene (C₆H₅-CH₂CH₃).

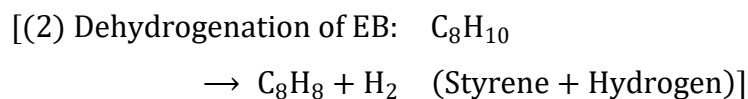
- Simplified reaction [39]:



2. Styrene production

Dehydrogenation of ethylbenzene (C₈H₁₀) to styrene (C₆H₅-CH=CH₂). Occurs at c.600-650 °C, often with iron oxide-based catalysts.

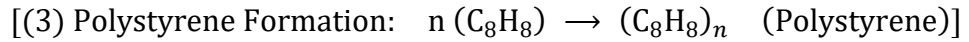
- Simplified reaction [40]:



3. Polystyrene formation

Styrene undergoes addition (chain-growth) polymerization to form polystyrene (PS).
No major by-products are released, as it's a direct polymerization of the monomer.

- Simplified reaction [40]:



Typical mass balance [40]:

- Styrene to PS: c.1 ton styrene $\rightarrow$ c.1 ton PS (near 1:1 under ideal conditions).
- Ethylbenzene to styrene: c.1.05 tons EB $\rightarrow$ c.1 ton styrene (to account for <100% conversion).
- Benzene + Ethylene to EB: c.0.77-ton benzene + c.0.28-ton ethylene $\rightarrow$ c.1 ton EB (again, near stoichiometric but slightly more in real practice).

3.5.4.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Alkylation (benzene + ethylene $\rightarrow$ ethylbenzene)	0.07	2.51	-3.10 (export)
Dehydrogenation of ethyl-benzene $\rightarrow$ styrene	0.22	1.68	6.19
Addition polymerisation of styrene $\rightarrow$ PS	0.37	0.53	0.01

Table 25 PS production energy consumption (unadjusted) [26]

Table 25 shows the unadjusted energy consumption of all the PS production sub-processes.

Sub-process	Electricity (GJ / t of PS)	Fuel (GJ / t of PS)	Steam (GJ / t of PS)
Alkylation (benzene + ethylene → ethylbenzene)	0.07	2.51	-3.10
Dehydrogenation of ethyl-benzene → styrene	0.22	1.68	6.19
Addition polymerisation of styrene → PS	0.37	0.53	0.01

Table 26 PS production energy consumption (adjusted for mass balance)

Table 26 shows the adjusted energy consumption of all the PS production sub-processes scaled by using the previously described mass balances.

3.5.4.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ /t of intermediate products]	CO ₂ (energy use) [t CO ₂ /t of intermediate products]
Alkylation (ethylene + benzene → ethyl-benzene)	0.00	0.01
De-hydrogenation (ethyl-benzene → styrene)	0.05	0.58
Addition polymerisation (styrene → PS)	0.03	0.15

Table 27 PS production emissions (unadjusted) [26]

Table 27 shows the unadjusted emissions of all the PS production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PS]	CO ₂ (energy use) [t CO ₂ /t of PS]
Alkylation (ethylene + benzene → ethyl-benzene)	0.00	0.01
De-hydrogenation (ethyl-benzene → styrene)	0.05	0.58
Addition polymerisation (styrene → PS)	0.03	0.15

Table 28 PS production energy consumption (adjusted for mass balance)

Table 28 shows the adjusted emissions of all the PS production sub-processes scaled by using the previously described mass balances.

3.5.5 PE PRODUCTION

Polyethylene (PE) is produced from Ethane. When compared to some of the other processes reviewed in this project, PE production is much simpler as it only entails one step to the process.

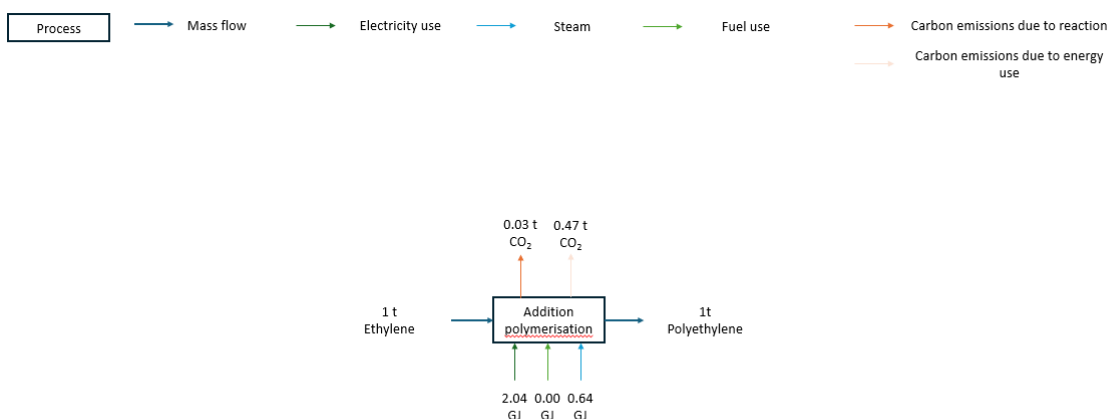


Figure 11 PE production process (own elaboration)

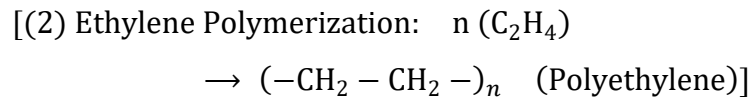
Figure 11 summarizes this process schematically, including mass input to output ratios, energy consumption and emissions associated with the process.

3.5.5.1 Mass balance

1. Ethylene Polymerization (Ethylene → Polyethylene)

Ethylene undergoes addition (chain-growth) polymerization under specific temperature/pressure conditions, often with a catalyst (e.g., Ziegler-Natta, metallocene, or Phillips catalyst) [40]. The polymerization forms long $-\text{CH}_2-\text{CH}_2-$ chains, yielding polyethylene (PE).

- Simplified reaction [40]:



2. Typical Mass Balance [40]:

- c.1.0 ton of ethylene yields c.1.0 ton of PE under near-ideal conditions (no significant by-products).
- Ethane to ethylene requires slightly more than 1 ton of ethane per ton of ethylene (depending on cracker efficiency and by-product yields). Real processes often achieve 80-90% ethane conversion per pass, with unreacted ethane recycled.

3.5.5.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Addition polymerisation (ethylene → PE)	2.04	0.00	0.64

Table 29 PE production energy consumption (unadjusted)[26]

Table 29 shows the unadjusted energy consumption of all the PE production sub-processes.

Sub-process	Electricity (GJ / t of PE)	Fuel (GJ / t of PE)	Steam (GJ / t of PE)
Addition polymerisation (ethylene → PE)	2.04	0.00	0.64

Table 30 PE production energy consumption (adjusted for mass balance)

Table 30 shows the adjusted energy consumption of all the PE production sub-processes scaled by using the previously described mass balances.

3.5.5.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ /t of intermediate products]	CO ₂ (energy use) [t CO ₂ /t of intermediate products]
Addition polymerisation of ethylene → PE	0.03	0.47

Table 31 PE production emissions (unadjusted)[26]

Table 31 shows the unadjusted emissions of all the PET production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PE]	CO ₂ (energy use) [t CO ₂ /t of PE]
Addition polymerisation	0.03	0.47

Table 32 PE production emissions (adjusted for mass balance)

Table 32 shows the adjusted emissions of all the PE production sub-processes scaled by using the previously described mass balances.

3.5.6 PP PRODUCTION

Polypropylene (PP) is produced from Propylene via a simplified 1-step process

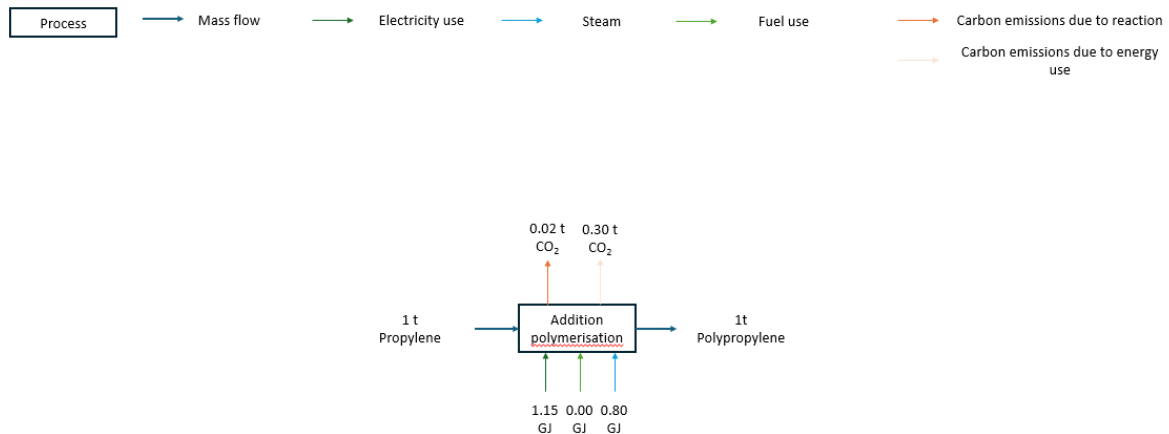


Figure 12 PP production process (own elaboration)

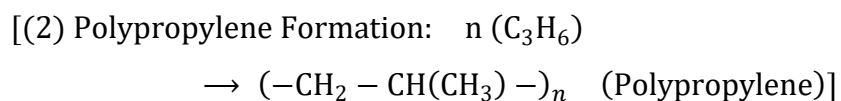
Figure 12 summarizes this process schematically, including mass input to output ratios, energy consumption and emissions associated with the process.

3.5.6.1 Mass balance

1. Polymerization (Propylene → Polypropylene)

Propylene undergoes addition (chain-growth) polymerization, typically in the presence of a Ziegler-Natta or metallocene catalyst [41]. The reaction forms long –CH₂–CH(CH₃)– chains, yielding polypropylene (PP).

- Simplified reaction [41]:



2. Typical Mass Balance [41]

- 1 ton of propylene can yield c.1 ton of polypropylene, assuming high conversion and minimal byproducts.

- Real processes often achieve > 95% conversion per pass, with unreacted propylene recycled.

3.5.6.2 Energy balance

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Addition polymerisation of ethylene	2.04	0.00	0.64

Table 33 PP production energy consumption (unadjusted) [26]

Table 33 shows the unadjusted energy consumption of all the PP production sub-processes.

Sub-process	Electricity (GJ / t of intermediate products)	Fuel (GJ / t of intermediate products)	Steam (GJ / t of intermediate products)
Addition polymerisation (propylene → PP)	1.15	0.00	0.80

Table 34 PP production energy consumption (adjusted for mass balance)

Table 34 shows the adjusted energy consumption of all the PP production sub-processes scaled by using the previously described mass balances.

3.5.6.3 Emissions balance

Sub-process	CO ₂ (reaction) [t CO ₂ / t of intermediate products]	CO ₂ (energy use) [t CO ₂ / t of intermediate products]

Addition polymerisation of propylene → PP	0.02	0.30
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Table 35 PP production emissions (unadjusted) [26]

Table 35 shows the unadjusted emissions of all the PP production sub-processes.

Sub-process	CO ₂ (reaction) [t CO ₂ /t of PP]	CO ₂ (energy use) [t CO ₂ /t of PP]
Addition polymerisation	0.02	0.30

Table 36 PP production emissions (adjusted for mass balance)

Table 36 shows the adjusted emissions of all the PP production sub-processes scaled by using the previously described mass balances.

3.5.7 ON-PURPOSE PROCESSES

On-purpose processes are processes used within the industry to convert excess intermediate to other more demanded compounds. For this project, these processes will serve as a balancing agent, to ensure that the production ratios across the value chain are realistic and that excess intermediate compounds can be transformed into more valuable compounds for the model. Given the low relevance of these processes, the description will be less detailed and will involve more high level data.

With regards to modelling, they won't be considered to have CAPEX and OPEX costs that serve for capacity building, just mere transformative processes with mass, energy and emissions associated to them.

3.5.7.1 Toluene Hydrode-alkylation (HDA)

Hydrode-alkylation converts surplus toluene and a small amount of hydrogen into benzene in a catalytic fixed-bed reactor operating at 610 – 700 °C and 30 – 45 bar. The strongly exothermic reaction mixture then goes through a flash, gas recycle (H₂/CH₄), and three

distillation columns to obtain 99.9 wt % benzene. This technology accounts for ~25 % of global benzene supply [24].

Global reaction: $C_7H_8 + H_2 \rightarrow C_6H_6 + CH_4$

Stream	kg benzene t ⁻¹	Note
Toluene	1,180	Stoichiometric, 97 % overall Bz selectivity; unconverted Tol recycled
Hydrogen	26	After 80–90 % gas recycle; make-up 2–3 wt % of fresh Tol feed
→ Benzene (product)	1,000	99.9 wt %
→ Methane (by-product)	206	Fired in site fuel system or sold as fuel gas
Heavy by-products (diphenyl etc.)	12	Purge to control build-up

Table 37 HDA mass balance [24]

Table 37 shows the estimated mass balance of relevant compounds.

Sub-process	Electricity (GJ)	Fuel (GJ)	Steam (GJ)
Total HDA	0.21	2.85	1.1

Table 38 HAD energy balance [24]

Table 38 shows the energy consumptions associated to the HDA process.

3.5.7.2 Propylene recovery FCC

Fluid-Catalytic Cracking (FCC) of vacuum gas-oil (VGO) is routinely swung to maximize C_3 = yield by raising riser temperature, adding ZSM-5 additives and, in the gas plant, deep-cut fractionation. Reporting an 18–20 wt % propylene on fresh feed for VGO feeds.

Stream	t per t PGP
Fresh VGO feed	5.5
→ Propylene (PGP)	1.00

Table 39 Mass balance Propylene recovery FCC [24]

Table 39 shows the mass balance of relevant compounds for FCC propylene recovery process.

Sub-process	Electricity (GJ)	Fuel (GJ)	Steam (GJ)
Total	0.60	5.35	−0.65

Table 40 Propylene recovery FCC energy consumption [24]

Table 40 shows the energy consumptions associated to the FCC propylene recovery process

3.6 MANAGING PLASTICS WASTE

Plastic waste can be managed in three main ways, either it is recycled through a variety of processes, or it is burnt as fuel to produce energy. For the purpose of this project, recycling and energy recovery methods are of great interest to help model the end-of-life management of plastics.

For each of the final compounds included in the model, the best recycling processes will be selected from academic research, and they will be modelled by their emissions and energy flows.

3.6.1 RECYCLING

The three main methods for plastics recycling are mechanical, physical and chemical recycling. Each are based on the alteration of different properties of the plastics waste to produce intermediate recycled inputs for the production of the same chemical compound.

- Mechanical recycling involves the physical reprocessing of plastic waste through steps such as sorting, washing, shredding, melting, and re-extruding to produce plastic pellets (regranulate) [42]. This method relies heavily on clean, homogeneous input waste; the quality of the recycled plastic is typically lower than that of virgin plastic, which limits its reuse in high-performance applications [42].
- Chemical recycling breaks down plastic polymers into their basic chemical building blocks—monomers, fuels, or feedstocks—through processes like pyrolysis, gasification, or depolymerization. It is suitable for mixed or contaminated plastics that are difficult to mechanically recycle, and the resulting outputs can be of virgin-like quality [42].
- Physical recycling is sometimes considered a hybrid between mechanical and chemical methods. It involves solvent-based dissolution of plastics. This process purifies the polymer without breaking its molecular structure, enabling the recovery of high-purity plastics suitable for demanding applications. Physical recycling is still under development and not yet widely implemented at industrial scale [43].

3.6.2 ENERGY RECOVERY

Energy recovery is a waste management method that involves the incineration of plastic waste to generate electricity and/or heat. Unlike recycling, where the goal is to recover materials, energy recovery focuses on extracting the energy content of plastics, which are derived from fossil fuels and therefore have a high potential as fuel [44]. The process typically involves combustion in specialized waste-to-energy plants, where plastics are burned under controlled conditions. The resulting heat is used to produce steam that drives turbines for electricity generation or provides direct heating through district heating systems. Although energy recovery can reduce the volume of plastic waste and divert it from landfills,

it is generally considered the least preferred option in the waste hierarchy after recycling. This is because it results in the complete loss of material value and emits significant amounts of carbon dioxide and other pollutants, including those from fossil-based polymers [44]. Some of these impacts are partially offset by the substitution of conventional fossil fuels in power generation, but the net climate benefit is often inferior to recycling—especially as energy systems become increasingly decarbonized. Additionally, energy recovery produces residues like fly ash and bottom ash, which require further treatment or landfilling.

3.6.3 SELECTION OF RECYCLING PROCESSES

To quantify the energy and emissions characteristics of every recycling method, this project has chosen to analyze the existing literature and choose the method that most suitably—defined as a combination of quality output, real world application of technology—represents the recycling process for each product that appears in the model (i.e. PET, PE, PP, PVC, PUR and PS). This approach yields several benefits over a more generic approach where for example, mechanical recycling is characterized in the same way for every product, which are mainly:

- Technology choice: Mechanical PET or PE is almost an order-of-magnitude cleaner than PS pyrolysis or PUR glycolysis [43]. For this reason, individual election of processes represents reality better.
- Material quality constraints: Dissolution gives food-contact PP or high-spec PVC, whereas conventional mechanical recycling cannot [43]. Describing the processes specifically for each product, guarantees a better approximation to reality.

3.6.4 ENERGY AND EMISSIONS BALANCES

Polymer	Most suitable recycling route	Energy use	CO ₂ emissions	Sources

PP	Super-critical-propane dissolution (physical recycling)	1.1 GJ t ⁻¹	0.32 t CO ₂ eq t ⁻¹	[45]
PET	Conventional mechanical bottle-to-bottle recycling	15 GJ t ⁻¹	0.90 t CO ₂ eq t ⁻¹	[46]
PE (HDPE/LDPE)	Mechanical re-granulation	4.1 - 8.6 GJ t ⁻¹ (6.4 used in model)	0.28 - 0.53 t CO ₂ eq t ⁻¹ (0.4 used in model)	[47]
PVC	Selective dissolution process	25.7 GJ t ⁻¹	1.94 t CO ₂ eq t ⁻¹	[48]
PS	Catalytic pyrolysis to styrene monomer	10 GJ t ⁻¹	2.91 t CO ₂ eq t ⁻¹	[48]
PUR (flexible & rigid foams)	Split-phase glycolysis	c. 5 GJ t ⁻¹	3.8 - 5.6 t CO ₂ eq t ⁻¹ (4.7 used in model)	[49]

Table 41 Recycling energy consumption and emissions

Table 41 summarizes the energy consumption and emissions ratios that will be used for the model. It is necessary to note that these emissions and energy usage will come at a one-to-one mass ratio of input to output of plastics, leaving process efficiencies aside, simplifying the process. This means that in terms of mass, recycling will be modelled as giving back the monomers and other compounds of which the plastic was originally made.

3.7 DECARBONIZATION PATHWAYS

After analyzing each of the processes that make up the plastics value chain, and with the goal of this project in mind—studying the petrochemical industry path to climate neutrality by 2050 in Spain—this project now aims to study and characterize the main levers that will push the industry to climate neutrality for the following years. To do this, an assessment has been developed, quantifying the impact of each of these levers so that this theoretical assessment can be transferred to the model in the following stages of execution.

The study has been developed by grouping the alternatives into three distinct categories which will be explained in the following sections:

- Process energy substitution
- Feedstock decarbonization
- Other levers (mitigation, optimization, CCUS, efficiency measures)

In each of these ‘buckets’, the main levers found in the review literature will be characterized, meaning that even though the categories themselves are exhaustive, not all of the levers in each category will be described as this process would enlarge complexity and end up adding little to no value. The goal here is to capture the main levers that the industry will use in the upcoming years and decades.

3.7.1 PROCESS ENERGY SUBSTITUTION

In line with the description of the production processes, key levers have been identified for the substitution of fuel, electricity and steam consumption. Each lever is described in terms of what physically changes, the maximum percentage reduction it can deliver relative to a 2023 baseline, and a technology-readiness indicator that allows this project to quantify when these tools will be ready for use.

3.7.1.1 Fuel substitution

Fuel substitution refers to all the initiatives aimed at changing, reducing or remediating the effects of the fuel employed in plastics production processes.

Lever	Concept	CO ₂ -reduction potential	Technology Readiness Level (TRL)
Electrified furnaces (“e-cracker”)	Replace gas-fired coils in steam crackers with electric heating elements.	~ 90-95 % of emissions when powered by renewables.	TRL 6-7: Early commercial roll-out after 2030 [50]
Renewable-hydrogen combustion	Fire cracking furnaces, reformers or package boilers with low-emission H ₂ (pure or high-blend).	~ 60-90 % direct CO ₂ cut, depending on H ₂ origin & blend share.	TRL 7-8: multiple industrial pilots; expected commercial 2027-2035 [51].
Post-combustion CCS	Capture 85-95 % of flue-gas CO ₂ and store it geologically.	~ 70-90 % net reduction.	TRL 8: technology proven; deployment pace limited by CO ₂ -transport & storage build-out in late 2020s.
Feedstock recycling	Already discussed in the previous section		

Table 42 Fuel consumption decarbonization levers

Table 42 summarizes the main levers that have been identified in this category. Electrified furnaces (“e-cracker”) replace the fossil-fuel burners in a steam cracker with electric heating elements powered by low-carbon electricity, eliminating direct combustion CO₂ emissions. Renewable-hydrogen combustion swaps natural-gas burners for ones that burn hydrogen produced from renewable power (green H₂); the hydrogen flame provides the same high-temperature heat but releases only water vapor at the point of use. Post-combustion CCS adds capture units to the flue-gas stream after traditional firing; the system strips CO₂ from

the exhaust, compresses it, and routes it for geological storage or utilization, allowing existing furnaces or boilers to keep running while cutting stack emissions.

3.7.2 ELECTRICITY USE

Electricity use refers to the levers identified that will decarbonize the energy consumed by plastics production processes in the form of electricity.

Lever	Concept	CO ₂ -reduction potential*	Technology Readiness Level (TRL)
Decarbonizing grid supply (IEA Net-Zero pathway)	Exogenous decline in grid emission factor as renewables share rises.	Up to 100 % of purchased-power emissions by 2050 in NZE scenarios.	Fully available, integration based on IEA scenarios towards net zero [3], [13].

Table 43 Electricity usage decarbonization levers

Table 43 shows the only lever that has been deemed relevant for the scope of this project. Decarbonizing grid supply (IEA Net-Zero pathway) refers to shifting the electricity mix rapidly toward near-zero-carbon sources—largely renewables, nuclear, and fossil plants with CCS—so the power drawn by petrochemical sites (for e-crackers, compressors, utilities, etc.) carries minimal upstream CO₂, enabling electrification measures to deliver full emissions cuts.

Other levers such as renewal of compressors and other electricity consuming equipment were studied but concluded to be not relevant enough.

3.7.3 STEAM USE

Steam use refers to the levers identified that will decarbonize the energy consumed by plastics production processes in the form of steam.

Lever	Concept	CO ₂ -reduction potential*	Technology Readiness Level (TRL)
Electric boilers	Convert fossil steam generation to resistive boilers.	~100 % if supplied with renewable power; ~35 % with average 2025 EU grid.	Fully available, integration based on IEA scenarios towards net zero [3], [13].

Table 44 Steam use decarbonization levers

Once again, Table 44 shows the only relevant lever to be included. Electric boilers will replace fossil-fired steam boilers with electrode/resistance units powered by low-carbon electricity, generating process steam without on-site combustion CO₂ emissions.

3.8 SUMMARY TABLES OF PLASTICS PRODUCTION PROCESSES

Process	Feedstock inputs (t / t of feed)	Product outputs (t / t of feed)	Electricity (GJ / t of feed)	Fuel (GJ / t of feed)	Steam (GJ / t of feed)	Reaction CO ₂ (t / t of feed)	Energy CO ₂ (t / t of feed)
Steam cracking - Group A	0.349 t Ethane 0.185 t Propane 0.045 t n-Butane 0.415 t Naphtha	0.503 t Ethylene 0.116 t Propylene 0.049 t Aromatics 0.038 t Butadiene 0.117 t C4/C5 & fuel-oil 0.017 t H ₂ 0.017 t CH ₄	0.02	2.06	-	-	1.05
Steam cracking - Group B	(same mix)	0.503 t Ethylene 0.116 t Propylene 0.049 t Aromatics 0.038 t Butadiene 0.117 t C4/C5 & fuel-oil 0.017 t CH ₄	0.051	3.67	-	-	1.03
Catalytic reforming	1.000 t Heavy naphtha	0.918 t Reformate 0.0696 t H ₂ 0.0104 t LPG 0.0017 t Fuel-gas	0.24	1.46	-	-	0.123

Table 45 Summary of monomer production key parameters

Polymer	Feedstock input (t / t of product)	Product output (t / t of product)	Electricity (GJ / t of product)	Steam (GJ / t of product)	Fuel (GJ / t of product)	Reaction CO ₂ (GJ / t of product)	Energy CO ₂ (GJ / t of product)
Polypropylene (PP)	1 t Propylene	1.00	1.15	0.80	0.00	0.02	0.30
Polystyrene (PS)	0.231 t Ethylene + 0.819 t Benzene	1.00	0.66	3.10	4.72	0.08	0.74
Polyethylene terephthalate (PET)	0.230 t Ethylene + 0.640 t p-Xylene	1.00	2.59	6.38	3.35	0.36	1.31
Polyvinyl chloride (PVC)	0.450 t Ethylene	1.00	1.30	2.31	3.60	0.11	0.65
Polyurethane (PUR)	0.052 t Toluene + 0.830 t Epoxy	1.00	1.84	1.77	1.98	0.04	0.57
Polyethylene (HDPE / LDPE / LLDPE)	1 t Ethylene	1.00	2.04	0.64	0.00	0.03	0.47

Table 46 Summary of polymer production key parameters

Polymer	Feedstock input (t / t of product)	Product output (t / t of product)	Electricity (GJ / t of product)	Steam (GJ / t of product)	Fuel (GJ / t of product)	Reaction CO ₂ (GJ / t of product)	Energy CO ₂ (GJ / t of product)
High-propylene FCC revamp (Polymer- grade propylene)	5.5 t VGO	1.00	0.60	-0.65	5.35	0.80	0.33
HDA – Hydro-de- alkylation (Benzene)	1.18 t toluene	1.00	0.21	1.10	2.85	0.00	0.23

Table 47 Summary of on-purpose processes

Chapter 4. MODELLING THE PETROCHEMICAL

INDUSTRY

After deep diving into the processes of the petrochemical industry, the goal of this project is now to transcribe these mass, energy and emissions flows that have been deduced, to the equations that will be the core of the linear optimization model.

To do this, first the methodology and scope assumptions of the model will be explained, finally the model itself will be developed with its corresponding objective and constraints functions.

4.1 METHODOLOGY

This work builds a forward-looking optimization model of a petrochemical complex whose purpose is to chart the least-cost pathway from today's asset base to a low-carbon fleet. First, the scope: the model spans the six main polymers produced on site (PE, PP, PVC, PUR, PS and PET) plus all upstream units that supply olefins, aromatics and utilities; it also embeds every decarbonization lever currently under discussion—electric boilers, green-hydrogen furnaces, CCS retrofits and a fully-electric steam cracker. The time horizon runs in annual steps from 2025 to 2050.

Second, data collection and parametrization: every numerical input is stored in an Excel workbook. A Parameters sheet holds scalar settings (e.g., discount rate, equipment lifetimes) and staircase series for prices, demands and emission factors; a Master Matrix sheet provides the α -coefficients that map each technology to its material and energy flows. During the read-in phase the code trims those sheets to a curated list of technologies and commodities, forward-fills any missing future values, converts percentage rows into absolute €/t·yr numbers, and tags each technology as Base, Increment or pure Procurement. Existing

capacity is imported together with a synthetic “legacy CAPEX” stream so that sunk investments continue to amortize inside the objective.

Finally, formulation: the cleaned data feeds a Pyomo model whose decision variables are annual throughputs, new-build capacity and resulting name-plate capacity stock. Constraints enforce material balances, capacity limits, ramp-up ceilings for every decarbonization family, and a $\geq$ -demand rule for each finished polymer. The objective function minimizes the net-present cost of raw-material purchases, utilities, CAPEX annuities (new and legacy), fixed O&M and all CO₂ liabilities—direct, grid and fuel-related—discounted back to 2025. With this structure in place, the optimizer is free to choose what to build, when to build it and how intensely to exploit every asset in every year, while respecting the physical and policy boundaries encoded in the parameters.

Development is carried out in Visual Studio Code, which provides linting, interactive debugging and a robust Git interface; the analytical core is written in Python, chosen for its rich scientific-computing ecosystem and seamless data handling with pandas. Optimization is handled by Pyomo, whose algebraic modelling language allows us to express complex constraints and call industry-grade solvers (Gurobi in this case) without sacrificing readability. This outside-in stack—VSCode for productivity, Python for data wrangling, Pyomo for mathematical rigour—gives a transparent, reproducible and easily extensible modelling platform.

4.2 LINEAR OPTIMIZATION MODEL

A linear optimization model in essence is a mathematical tool for picking the best plan when you have limited resources and clear, straight-line trade-offs. One lists what one wants to achieve—say, minimize total cost—and one lists the rules you must obey, such as capacity limits or environmental caps. The outcome tells one, in the most economical way possible, how much to make, buy, or invest to reach one’s goal without breaking any constraints.

As in any other linear optimization model, this thesis now explains the main parameters, variables and equations that will go into the creation of the objective function and constraints equations.

In this project, the goal of the model is to represent the petrochemical industry, focusing on the production of plastics, and developing a model to evaluate sustainability-related topics such as its decarbonization pathways, or whether the targets set for neutrality by 2050 are achievable.

4.2.1 PARAMETERS

Before formalizing the optimization problem, it is useful to step back and describe the numerical levers that appear inside every term of the model. All of these quantities are fixed inputs that the optimizer cannot change, only react to. For explanatory purposes, they have been grouped into three families: economic, energy, and sustainability-related. Additionally, throughout the whole model, time and the different plastic production methods will be modelled through the following nomenclature:

- Time – $t \in T$ is a discrete calendar year. $T = \{2025, \dots, 2050\}$.
- Process routes – $g \in G$ is every row of the Master-Matrix sheet:
 - Base routes that already exist in the reference plant, e.g., PE (HD/LD/LL) or Steam cracking A.
 - Increment routes that sit on top of a base unit and apply a decarbonization lever, e.g., PE (HD/LD/LL)_H2, PVC_CCS, or the stand-alone Steam cracking A_Ecracker.
 - PROC routes that represent pure procurement (outside-battery-limit purchases), e.g., Naphtha_Procurement, Electricity_Procurement.

- Commodities – $i \in I$ include every reagent, intermediate or utility that appears in at least one α -coefficient: hydrocarbon feeds, utilities (steam, NG, H₂, electricity), finished polymers, and bookkeeping items such as CO₂ (reaction).
- Families – Decarbonization levers are grouped into the suffixes H₂, CCS, E-boiler, E-cracker. These four strings appear throughout the parameter logic to align CAPEX, OPEX and ramp fractions.

This structure has been chosen as it allows for a general matrix to be described, that includes every process route and its corresponding input and outputs. This way, all of the data will be compiled into a matrix when the programming phase is reached.

4.2.1.1 Economic and commodity parameters

Every euro that enters or leaves the objective function is driven by at least one of the following numbers.

- Real discount rate – A user-supplied WACC (cell `real_WACC` on the Parameters sheet), which is calculated using a nominal rate minus inflation, feeding the discount factor which multiplies every term of the NPV objective.
- Commodity purchase prices – For every procurement route $g \in \text{PROC}$ the model reads a staircase series (`<commodity>_price_2025, 2030, ...`), forward-fills the last known knot and stores it as €/t (chemicals) or €/GJ (utilities).
- Carbon price – `CO2_price_YYYY` gives a €/tCO₂ trajectory used for:
 - direct stack emissions (CO₂ (reaction)),
 - grid-electricity emissions (through `grid_EF_YYYY`),
 - fuel & steam emissions (using Natural Gas_EF and Hydrogen_EF) net of any CCS capture.

- Grid decarbonization – grid_EF_yyyy (t CO₂/GJ) encodes the CO₂ intensity of the marginal MWh. A cleaner grid therefore reduces both the indirect carbon penalty and the attractiveness of on-site E-boilers/E-crackers.
- Polymer demand outlooks – Each finished plastic has its own staircase demand vector demand_<polymer>_yyyy that enters the balance. The optimizer must at least meet, never exceed, those external tons.

4.2.1.2 Investment and operating parameters

These numbers link the model to building capacity costs as well as investment in new technologies for existing capacity.

- Unit CAPEX trajectories – For every $g \in \text{BASE} \cup \text{INCR}$ the model looks for
 - Exact data e.g. CAPEX_2030_PE (HD/LD/LL)_H2, for every process technology along the time horizon of the simulation.
 - Family fallbacks CAPEX_2030_H2 if no polymer-specific row exists.
- Capital is annualized with a project-specific lifetime Life_<tech> (or suffix catch-all Life_H2, Life_CCS, ...) and the same real WACC.
- Fixed O&M – Analogous logic under the OPEX_yyyy_* prefix turns %-of-CAPEX lines into absolute €/t-yr. OPEX is applied to the installed capacity, not to the actual throughput.
- Existing capacity – Cap0_<tech> initialize each Base or Increment line. Three “vintages” (15, 10, 5-year-old) are assumed so that historical CAPEX annuities continue to burden the P&L until their individual end-of-life.
- Ramp fractions – Rows like Ramp_2030_Eboiler = 0.40 cap the name-plate capacity of all Increment rows that share the same polymer prefix and lever suffix. This enforces a physically plausible roll-out path for CCS retrofits, electric boilers, green-H₂ furnaces or electric crackers.

- Learning curves – The spreadsheet, not the Python code, embodies any assumed cost decline; once the new staircase is entered, the model treats it deterministically.

4.2.1.3 Energy & sustainability parameters

- Direct process emissions – The Master-Matrix column CO₂ (reaction) provides stoichiometric tCO₂ per ton of throughput for cracking or reforming steps. These tons are priced in full.
- Fuel & steam emissions – Emission factors Natural Gas_EF, Hydrogen_EF multiplied by procurement flows create a second CO₂ channel. A CCS retrofit on the main PE furnace acts as a multiplier that reduces the NG total emissions by a factor of the CCS that has been installed with respect to the total technology production.
- Electricity emissions – Grid intensity grid_EF_t × electricity procurement merges seamlessly into the same carbon account.

4.2.1.4 Stoichiometry-related parameters (α -matrix)

Before any optimization takes place, every technology is reduced to a single row in the α -matrix: a vector of fixed coefficients that translates one ton of reference output into the concurrent inputs, co-products and reaction emissions.

The α -matrix is the basis for the programming and reduction of the model equations.

- Sign convention. Positive numbers denote net production; negative numbers net consumption. Thus, Steam cracking A produces 0.50 t ethylene and consumes –2.06 t NG per ton of olefins, while Electricity_Procurement has a +1 in the electricity column and zeros elsewhere.
- Row taxonomy.
 - Base rows: existing base processes for monomer and polymer production
 - Increment rows: retrofitted levers (E-boilers, CCS, H₂ and E-crackers)
 - PROC rows: procurement of raw materials and utilities

- The optimizer can mix any Increment with its corresponding Base but must buy or sell through the PROC rows to close the balances.
- Utility-switch levers. For every polymer, the Eboiler row flips equal magnitudes between the Steam and Electricity columns (e.g. $-0.80 \leftrightarrow +0.80$ t steam-eq t^{-1} in PP_Eboiler). Likewise, the H₂ rows replace the NG entry in the Base row with an equal negative coefficient in Hydrogen and a positive one in Natural Gas, signaling displacement rather than additive use. These clean one-for-one substitutions ensure that the model can rebalance the procurement flows algebraically without touching anything else.
- CCS capture logic. Increment rows suffixed “_CCS” reverse the sign of the CO₂ (energy) coefficient found in the Base row. For Steam-cracking A, the base emits +1.05 t CO₂; the CCS row carries -1.05 t CO₂, meaning one ton of Increment fully neutralizes one ton of Base emissions while leaving all material flows unchanged.
- E-cracker abstraction. The generic Ecracker row withdraws -2.06 GJ electricity and returns +2.06 GJ NG (fuel-gas), cancelling the furnace duty in the conventional cracker; its CO₂ columns are zero because the grid factor is handled elsewhere.

Mass & energy sanity. No row shows “free” material or energy creation: every positive credit is backed by a stoichiometrically plausible negative debit.

4.2.2 OBJECTIVE FUNCTION

$$\text{PurchaseCost}_t = \sum_{g \in \text{PROC}} c_{t,g} P_{t,g} \quad (1)$$

$$\text{CO2Cost}_t^{\text{direct}} = \left(\sum_{g \in G} \sum_{i \in \text{CO2}} \alpha_{g,i} P_{t,g} \right) p_t^{\text{CO2}} \quad (2)$$

$$\text{CO2Cost}_t^{\text{elec}} = P_{t,\text{Electricity_Procurement}} EF_t^{\text{elec}} p_t^{\text{CO2}} \quad (3)$$

$$\text{CO2Cost}_t^{\text{fuel+steam}} = P_{t,\text{Natural Gas_Procurement}} EF_t^{\text{NG}} p_t^{\text{CO2}} \quad (4)$$

$$\text{CapCost}_t = \sum_g \text{CAPEX}_{t,g} \frac{r(1+r)^{n_g}}{(1+r)^{n_g} - 1} \text{BuildCap}_{t,g} \quad (5)$$

$$\text{CapCost}_t^{\text{legacy}} \quad (6)$$

$$\text{FOM}_t = \sum_g \text{OPEXunit}_{t,g} \text{Cap}_{t,g} \quad (7)$$

$$\begin{aligned} \text{Total}_t &= \text{PurchaseCost}_t \\ &+ \text{CO2Cost}_t^{\text{direct}} \\ &+ \text{CO2Cost}_t^{\text{elec}} \\ &+ \text{CO2Cost}_t^{\text{fuel+steam}} \\ &+ \text{CapCost}_t \\ &+ \text{FOM}_t \\ &+ \text{CapCost}_t^{\text{legacy}} \end{aligned} \quad (8)$$

$$\min \sum_{t \in T} DF_t \text{Total}_t \quad (9)$$

Term	Role	Meaning of term
$\sum_{g \in \text{PROC}} c_{t,g} P_{t,g}$	Raw material & utility purchases	- $c_{t,g}$ – purchase price in period t (“feedstock price × multiplier” or “electricity price”) - $P_{t,g}$ – total of the procurement rows (tons or GJ)
$\left(\sum_{g \in G} \sum_{i \in \text{CO}_2} \alpha_{g,i} P_{t,g} \right) p_t^{\text{CO}_2}$	Direct-process CO ₂ cost	- $\alpha_{g,i}$ – CO₂ emitted per ton of activity (three separate matrix columns) - $P_{t,g}$ – throughput of technology g - $p_t^{\text{CO}_2}$ – carbon price
$P_{t,\text{Electricity_Procurement}} EF_t^{\text{elec}} p_t^{\text{CO}_2}$	Indirect grid-CO ₂ cost	- $P_{t,\text{Electricity_Procurement}}$ – grid-electricity purchased (GJ) - EF_t^{elec} grid-emission factor (t CO₂/GJ)
$P_{t,\text{Natural Gas_Procurement}} EF_t^{\text{NG}} p_t^{\text{CO}_2}$	Indirect fuel and steam-CO ₂ cost	- $P_{t,\text{Natural Gas_Procurement}}$ – natural gas purchased (GJ), boilers are modelled as purely natural gas based

		- EF_t^{NG} natural gas-emission factor (t CO₂/GJ)
$CapCost_t^{legacy}$	Legacy annualized capital cost of year 0 installed fleet	
$\sum_g CAPEX_{t,g} \frac{r(1+r)^{n_g}}{(1+r)^{n_g}-1} BuildCap_{t,g}$	Annualized capital cost	- $CAPEX_{t,g}$ – unit investment cost (€/t capacity · y) after learning curve - $BuildCap_{t,g}$ – new capacity added in year t - $\frac{r(1+r)^{n_g}}{(1+r)^{n_g}-1}$ – capital-recovery factor using real discount rate r and lifetime n_g
$\sum_g OPEX_{unit,t,g} Cap_{t,g}$	Fixed O&M on existing capacity	- $OPEX\%_g$ – percentage in “OPEX (% of CAPEX)” column - $CAPEX_{t,g}$ – capital expenditure per ton of new capacity (€ / t)

		- $Cap_{t,g}$ – installed capacity in year t
$C_{t,g} * OPEX_{t,g}$	Fixed operating cost of the installed capacity	- $C_{t,g}$ – existing capacity (t) - $OPEX_{t,g}$ – fixed O&M cost per ton of capacity (€/t capacity) at any given period for any given group
DF_t	Time value of money	- $DF_t = \frac{1}{(1+WACC)^{t-t_0}}$
t_j	Period length	

Table 48 Objective function parameters

4.2.3 CONSTRAINTS

$$\sum_g \alpha_{g,i} * P_{t,g} \geq 0 \quad \forall i \in INT \cup EXT \quad (10)$$

$$\sum_g \alpha_{g,i} * P_{t,g} = D_{t,i} \quad \forall i \in DEM \quad (11)$$

$$P_{t,g} \leq Cap_{t,g} \quad \forall g \in Base, Increment \quad (12)$$

$$BuildCap_{t,g} \leq RampFrac_{t,g} * Cap_{t,base} \quad \forall g \quad (13)$$

$$Cap_{t,g} = Cap_{t-1,g} + BuildCap_{t,g} \quad \forall g \quad (14)$$

$$P_{t,\Delta g} \leq P_{t,g} \quad \forall g \in Increment \quad (15)$$

Constraint	Role	Meaning of terms
$\sum_g \alpha_{g,i} * P_{t,g} = D_{t,i} \quad \forall i \in DEM$	Meet polymer (end-product) demand in every year	- $\alpha_{g,i}$- output (+) or input (-) of commodity i by process g - $P_{t,g}$ - production of technology g in period t - $D_{t,i}$- Externally given demand for end-products (i.e., PET, PP...)
$\sum_g \alpha_{g,i} * P_{t,g} = 0 \quad \forall i \text{ group} \in INT \cup EXT$	Mass and energy balance for every intermediate and purchased feedstock or utility	- $INT \cup EXT$ references to i groups of intermediates and utilities
$P_{t,g} \leq Cap_{t,g} \quad \forall g \in Base, Increment$	Capacity limits on production – output cannot exceed the installed (or permitted) maximum	- $Cap_{t,g}$ - maximum feasible production due to limits on installed based capacity (t, g)

$Cap_{t,g}$ $= Cap_{t-1,g} + BuildCap_{t,g}$	Capacity evolution & utilization – installed capacity rolls forward with new builds. No retirement variable exists, the model is only able to use the capacity for its defined lifetime	- $Cap_{t,g}$ - installed capacity (t prod / period) - $BuildCap_{t,g}$ - new capacity (t)
$BuildCap_{t,g} \leq RampFrac_{t,g} * Cap_{t,base} \quad \forall g$	Maximum capacity built in any period –cannot exceed the capacity that exists in that period under a defined ramp constraint	- $RampFrac_{t,g}$ - maximum installable capacity per period (%) - $Cap_{t,base}$ - Proxy for capacity ramp constraint
$P_{t,\Delta g} \leq P_{t,g}$	Couples each decarbonization lever (e-cracker, H₂ furnace, CCS, e-boiler) to its parent unit so it is not possible to retrofit more than exists	- $P_{t,\Delta g}$ - production of decarbonization levers

Table 49 Constraints summary table

4.2.4 QUANTIFYING PARAMETERS

To finalize the planning phase before starting the programming phase of the project, it is necessary to quantify all the specific data points that the model requires (i.e., investment and operation costs (CAPEX and OPEX), carbon prices, raw materials prices, import prices, WACC, energy prices and others).

4.2.4.1 Feedstock prices

Feedstock prices are heavily influenced by international trade and the macroeconomic environment. The goal of this project is not to study the influence of the variance of feedstock prices on decarbonization, but to assess the feasibility of decarbonizing this sector through technological progress and initiatives that the industry should invest in the following decades and feedstock prices influence the ability to carry out these investments. For this reason, feedstock price variation is a critical factor and the methodology to estimate their prices until 2050 has been to pick a baseline price and elaborate a projection based on reference scenarios by the EU or other reputable sources. Additionally, whenever possible, CIF (Cost, Insurance, and Freight) prices have been extracted, referring to the total cost of goods delivered to the buyer's port, including the cost of the goods themselves, insurance, and freight charges.

Commodity	Price	Unit	Source
Naphtha	585	€/t	[52]
Propane	490	€/t	[53]
Ethane	215	€/t	[52]
Natural gas	11.4	€/GJ	[54]
Hydrogen	33.3	€/GJ	[13]
Propylene	900	€/t	[55]
Ethylene	950	€/t	[55]
Benzene	1,050	€/t	[55]
p-Xylene	860	€/t	[55]
Toluene	750	€/t	[55]

n-Butane	655	€/t	[55]
Epoxy	3,000	€/t	[55]

Table 50 Feedstock price data

Table 50 shows the estimated baseline prices as well as each of the sources for the values. Natural gas and hydrogen will be used as fuel and for this reason their units are €/GJ. Generally, values can be found in €/MWh, the transformation to €/GJ can be made simply dividing by 3.6.

	Naphtha (€/t)	Propane (€/t)	Ethane (€/t)	Natural gas (€/GJ)
2025	585	490	215	11.4
2030	673	564	247	11
2035	761	637	280	10
2040	807	676	297	10
2045	857	718	315	10
2050	907	760	333	10
Hydrogen (€/GJ)	Propylene (€/t)	Ethylene (€/t)	Benzene (€/t)	
33.3	900	950	1,050	
29	1,035	1,093	1,208	
24	1,170	1,235	1,365	
19	1,242	1,311	1,449	
15	1,319	1,392	1,538	
10	1,395	1,473	1,628	
p-Xylene (€/t)	Toluene (€/t)	Epoxy (€/t)	n-Butane (€/t)	
860	750	3,000	655	
989	863	2,670	753	
1,118	975	2,340	852	
1,187	1,035	2,010	904	
1,260	1,099	1,680	960	
1,333	1,163	1,350	1,015	

Table 51 Feedstock price projections

Table 51 shows the result of the feedstock price predictions for the 2025-2050 outlook. To elaborate this projection, the base prices have been multiplied by a factor that varies over time. This factor has been directly deduced from predictions by agencies or other sources, and to summarize what has been deduced, all hydrocarbon-derived compounds have been

estimated to have the same price path, and natural gas and hydrogen have been predicted through individual multipliers as their price will likely not be tied in a similar fashion.

Feedstock price multipliers			
	(€/t)	(€/GJ)	(€/GJ)
	Naphtha	Natural gas	Hydrogen
2025	1	1	1
2030	1.15	0.95	0.86
2035	1.3	0.90	0.72
2040	1.38	0.90	0.58
2045	1.47	0.90	0.44
2050	1.55	0.90	0.3

Table 52 Feedstock multipliers

Table 52 shows the multipliers with respect to the reference price. Naphtha can be taken as a proxy for all of the hydrocarbon-derived compounds.

4.2.4.2 Electricity and carbon prices

For electricity prices, the approach is different as electrification is considered to be one of the main decarbonization pathways for the industry. So, to include this effect, and to model specifically the progress that Spain will gain from decarbonizing the grid, electricity price projections have been included as well as the percentage of renewables that the grid averages at any given period. This percentage is relevant as this will have an effect in the overall emissions of the grid and in the electrification process of several equipment pieces in the industry (e.g., electric furnaces).

For carbon prices, the same approach is followed mainly due to the same reasons discussed for electricity.

Year	Electricity price (€/MWh)	EU-ETS carbon price (€/t CO ₂)
2025	154	26.5

2030	158	30
2035	158	50
2040	159	80
2045	160	120
2050	161	150

Table 53 Electricity and carbon prices [56]

As the PRIMES model used in the EU 2020 reference scenario does not provide electricity prices for the 5-year intervals, linear interpolation has been used to calculate the values used in these years (i.e., 2025, 2035...). Also, it is necessary to note, that the average after-tax wholesale price across EU Member States is used. PRIMES notes that national prices converge toward the EU average by 2030, meaning that the assumption of prices being valid for Spain is generally correct.

Table 53 summarizes the values retrieved in an initial approach, however this approach was deemed inappropriate for carbon prices, as the estimates were provided in 2021 and in 2025, carbon prices are already far exceeding those predicted ones. For this reason, a new data collection based on current IEA estimates has been elaborated.

Year	Carbon price (€/t CO₂)
2025	71.2
2030	140
2035	180
2040	205

2045	228
2050	250

Table 54 Final carbon price estimation [16]

Table 54 shows the final values retrieved. 2025 value was retrieved from the current carbon price as of July 2025, and the projection for the following years was either directly retrieved from the Global Energy and Climate Model [16] or interpolated if missing.

To implement the effect of the decarbonization of the grid into the model, a grid emissions factor has been modelled based on the predictions of the IEA.

Grid emisisions (% of baseline)	Grid emission factors (t CO ₂ / GJ)
100%	0.12
80%	0.10
60%	0.07
40%	0.05
20%	0.02
0%	0.00

Table 55 Grid emissions

Table 55 shows the results of the grid emissions as a percentage of the baseline and the grid emissions factor associated in the 2025-2050 outlook.

4.2.4.3 Decarbonization levers investment costs

Decarbonization option	Unit	CAPEX	OPEX	Source
Electrified steam-cracker	€/t of ethylene y ⁻¹	2,470	3 % CAPEX yr ⁻¹	[57]

furnace (“e-cracker”)				
Industrial furnace converted to H₂ firing	€/GJ y ⁻¹	2	c. 4% of CAPEX yr ⁻¹	[58]
Post-combustion CCS	€/t CO ₂ y ⁻¹	60 (capture only; additional 10 €/t for T&S)	4 – 6 % CAPEX yr ⁻¹ (5% used in model)	[59]
Industrial electric boiler	€/GJ y ⁻¹	3	2 % CAPEX yr ⁻¹	[60]

Table 56 Decarbonization levers investment costs

Table 56 describes the CAPEX and OPEX benchmarks used in the model for the year 2025. Next, the issue is to project these costs into the future and find out what their values will be in the following years running from 2025-2050 in 5-year intervals.

To do this, three main hypotheses have been used:

- For e-crackers, the IEA “Net-Zero Roadmap” [13]: uses typical midpoint learning rates for emerging industrial technologies (12 – 15 % per doubling of capacity). The conservative estimate of 12% every 5 years has been used for this project. For H₂ furnaces, the same hypothesis has been used, but the doubling has been estimated to occur at a lower pace of 10 years, this is mainly due to the technology readiness level that has been described in previous sections.
- For CCS, Global CCS Institute “2023 Status Report” [59]: suggests a c.35 % CAPEX drop for post-combustion capture by 2050 as projects scale. This value has been linearly interpolated through the years up to 2050.

- For electric boilers, they have been defined as already commercially available technology, so only a 10% cost reduction has been estimated by 2035, then the cost flattens.

Taking into account all of these factors, the values shown in Table 57 are computed:

	E-cracker (€/t of ethylene · y)	H2 furnaces (€/GJ · y)	CCS (€/t of CO2 · y)	E-boilers (€/GJ · y)
2025	2,000	2.0	70	3.0
2030	1,760	1.9	65	2.9
2035	1,549	1.8	61	2.7
2040	1,363	1.7	56	2.6
2045	1,199	1.6	52	2.4
2050	1,055	1.5	49	2.3

Table 57 Projection of CAPEX decarbonization costs

OPEX remains a fixed percentage of CAPEX, and for this reason, its values also vary over time. Table 58 shows the values computed.

	E-cracker (€/t of ethylene · y)	H2 furnaces (€/GJ · y)	CCS (€/t of CO2 · y)	E-boilers (€/GJ · y)
2025	60.00	0.08	3.50	0.06
2030	52.80	0.08	3.26	0.06
2035	46.46	0.07	3.03	0.05
2040	40.89	0.07	2.82	0.05
2045	35.98	0.06	2.62	0.05
2050	31.66	0.06	2.43	0.05

Table 58 OPEX decarbonization costs projections

4.2.4.4 Capacity growth costs

Capacity growth refers to all the production facilities that will be modelled. To supply for demand, a certain production capacity will be estimated, and based on demand and supply balances, the model will be able to decide whether to invest in new facilities or not. The methodology to quantify these parameters has been the same one as the one previously described for decarbonization levers characterization, although in this case simpler, as no technology readiness level has to be taken into consideration.

Capacity growth	Unit	CAPEX	OPEX	Source
Steam cracker (A)	(€/t of ethylene · y)	1,600	3% CAPEX yr ⁻¹	[57]
Steam cracker (B)	(€/t of ethylene · y)	1,600	4% CAPEX yr ⁻¹	[58]
Catalytic reforming	(€/t of reformat · y)	2,200	5% CAPEX yr ⁻¹	[59]
PP	(€/t of PP · y)	650	2% CAPEX yr ⁻¹	[60]
PS	(€/t of PS · y)	800	2% CAPEX yr ⁻¹	[60]
PET	(€/t of PET · y)	600	2% CAPEX yr ⁻¹	[60]
PVC	(€/t of PVC · y)	750	2% CAPEX yr ⁻¹	[60]
PUR	(€/t of PUR · y)	1,100	2% CAPEX yr ⁻¹	[60]
PE	(€/t of PE · y)	800	2% CAPEX yr ⁻¹	[60]

Table 59 Capacity growth costs

Table 59 shows the results of capacity growth costs for the different production facilities included in the model. As well as the operating cost of these facilities.

Additionally, to project the costs into the 2025-2050 outlook, a learning curve methodology has been followed, with the following learning rates for each capacity type, which are estimated, and based on the TRLs described in the previous chapter of the document.

Capacity expansion parameters					
			Steam cracker (A)	Steam cracker (B)	Catalytic reforming
Learning curve	(% / 5-years)		5%	5%	6%
PP	PS	PET	PVC	PUR	PE
2%	2%	2%	2%	2%	2%

Table 60 Capacity expansion learning curve projections

Table 60 summarizes the values employed in the model.

	Steam cracker (A)	Steam cracker (B)	Catalytic reforming	PP	PS	PET	PVC	PUR	PE
	(€/t of ethylene · y)	(€/t of ethylene · y)	(€/t of reformat · y)	(€/t of PP · y)	(€/t of PS · y)	(€/t of PET · y)	(€/t of PVC · y)	(€/t of PUR · y)	(€/t of PE · y)
2025	1,600	1,600	2,200	650	800	600	750	1,100	800
2030	1,520	1,520	2,068	637	784	588	735	1,078	784
2035	1,444	1,444	1,944	624	768	576	720	1,056	768
2040	1,372	1,372	1,827	612	753	565	706	1,035	753
2045	1,303	1,303	1,718	600	738	553	692	1,015	738
2050	1,238	1,238	1,615	588	723	542	678	994	723

Table 61 Capacity growth CAPEX projections

	Steam cracker (A)	Steam cracker (B)	Catalytic reforming	PP	PS	PET	PVC	PUR	PE
	(€/t of ethylene · y)	(€/t of ethylene · y)	(€/t of reformat · y)	(€/t of PP · y)	(€/t of PS · y)	(€/t of PET · y)	(€/t of PVC · y)	(€/t of PUR · y)	(€/t of PE · y)
2025	48.00	64.00	110.00	13.00	16.00	12.00	15.00	22.00	16.00
2030	45.60	60.80	103.40	12.74	15.68	11.76	14.70	21.56	15.68
2035	43.32	57.76	97.20	12.49	15.37	11.52	14.41	21.13	15.37
2040	41.15	54.87	91.36	12.24	15.06	11.29	14.12	20.71	15.06
2045	39.10	52.13	85.88	11.99	14.76	11.07	13.84	20.29	14.76
2050	37.14	49.52	80.73	11.75	14.46	10.85	13.56	19.89	14.46

Table 62 Capacity growth OPEX projections

Table 61 and Table 62 show the result of applying the learning rates for the capacity expansion and operation costs in accordance to expected learning curve percentages.

4.2.5 MODELLING PLASTICS DEMAND

In linear optimization models, particularly those aimed at understanding industrial processes like petrochemicals, accurate demand estimation is critical, because the model is supposed to be used for analyzing the most efficient and sustainable ways to allocate resources, select production routes, and reduce environmental impacts. If the demand forecast is inaccurate, the optimization process may lead to suboptimal decisions, potentially underestimating production capacities, overestimating resource allocation, or failing to meet future needs. Given that these decisions can have significant economic, environmental, and operational implications, ensuring that the demand inputs into such models are as accurate and representative as possible is essential for making informed decisions.

4.2.5.1 Hypothesis

The hypothesis underpinning the projected demand for plastics in Spain between 2025 and 2050 is based on several key assumptions, guided by trends observed in the petrochemical sector and broader economic and environmental factors. The hypothesis follows from an analysis of past data, including the market demand from Europe, and extrapolates it to the Spanish context, using available projections from reputable sources like Plastics Europe and Systemiq's Re-Shaping Plastics study [61], [62]. The objective is to develop a demand forecast that reflects both the historical growth patterns and expected shifts in the plastics industry, as well as the influence of key global trends such as sustainability regulations, technological advancements, and the increasing pressure for decarbonization.

- Base year demand (2025): The starting point for demand projections is derived from the current estimated consumption levels of various plastics in Spain. The demand is based on total plastics consumption in the European Union, with Spain accounting for approximately 7.5% of that demand [61]. In 2025, the projected demand for plastics in Spain is estimated to be approximately 3.9 million tons across six major polymer categories: polypropylene (PP), polystyrene (PS), polyethylene

terephthalate (PET), polyvinyl chloride (PVC), polyurethane (PUR), and polyethylene (PE) [61].

- Growth rate: The demand projection assumes a compound annual growth rate (CAGR) of about 0.8% over the 2025-2050 period [62]. This is a conservative estimate based on growth rates seen in European markets and global trends in plastics consumption.
- Polymer demand distribution: The distribution of demand among the different polymer types is expected to remain relatively constant over the 25-year period, in line with historical trends. While shifts in consumer preferences and industrial applications might alter this distribution, for the purposes of this forecast, the proportional demand among PP, PS, PET, PVC, PUR, and PE is assumed to remain similar to current levels, with minor adjustments based on anticipated trends.
- Market conditions and economic shocks: The forecast assumes steady economic conditions without significant economic crises. However, unforeseen disruptions—such as a global recession or a substantial increase in raw material prices—could impact demand. The model accounts for these uncertainties through a range of sensitivity analyses that explore different scenarios based on varying economic conditions.

4.2.5.2 Results

Demand

(t / year)		(t / year)		(t / year)	
PP		PS		PVC	
2025	647,000	238,000	207,000	445,000	
2030	675,000	248,000	215,000	463,000	
2035	703,000	259,000	225,000	483,000	
2040	733,000	270,000	234,000	504,000	
2045	764,000	281,000	244,000	525,000	
2050	797,000	293,000	254,000	547,000	

(t / year)		(t / year)	
PUR		PE	
214,000	936,000		
224,000	976,000		

233,000	1,017,000
243,000	1,060,000
253,000	1,105,000
264,000	1,152,000

Table 63 Plastics demand predictions

Table 63 summarizes the values employed in the model for plastics demand in Spain in the 2025-2050 outlook.

Chapter 5. MODEL VALIDATION

After configuring and programming the model, this thesis now assesses the effectiveness and inner workings of the model, elaborating a two-section description, firstly analyzing whether technically the model is behaving as expected, and secondly, comparing the results with real industry data to confirm or reject the validity of the results and to assess the proximity to reality of the model.

5.1 TECHNICAL CONSISTENCY

The first stage in any optimization model is a purely technical one: do the numerical results respect the hard constraints that have been encoded? Using the diagnostic work-book that has been embedded into the code, it is possible to tick through every rule in turn and show that the solver has behaved exactly as intended.

Results are shown in 5-year intervals because key parameters change every 5 years and so the intermediate years in 2025-2030 do not provide any insights into the model but rather ensures the consistency of the logic of the model itself be consistent with reality.

5.1.1 MASS BALANCES

year	polymer	Produced (t)	Demand (t)
2025	PE (HD/LD/LL)	936,000.00	936,000.00
2025	PET	207,000.00	207,000.00
2025	PP	647,000.00	647,000.00
2025	PS	238,000.00	238,000.00
2025	PUR	214,000.00	214,000.00
2025	PVC	445,000.00	445,000.00
2030	PE (HD/LD/LL)	976,000.00	976,000.00
2030	PET	215,000.00	215,000.00
2030	PP	675,000.00	675,000.00
2030	PS	248,000.00	248,000.00
2030	PUR	224,000.00	224,000.00
2030	PVC	463,000.00	463,000.00

2035	PE (HD/LD/LL)	1,017,000.00	1,017,000.00
2035	PET	225,000.00	225,000.00
2035	PP	703,000.00	703,000.00
2035	PS	259,000.00	259,000.00

Table 64 Polymer demand balance

year	comm	Net (t)
year	comm	net
2025	Ethylene	0.00
2025	Electricity	0.00
2025	Steam	0.00
2025	Natural Gas	0.00
2025	Naphtha	0.00
2025	n-Butane	0.00
2025	Propane	0.00
2025	Ethane	0.00
2025	Benzene	0.00
2025	p-Xylene	28,507.40
2025	Toluene	0.00
2025	Propylene	0.00
2025	Hydrogen	0.00
2025	Epoxy	0.00
2030	Ethylene	0.00
2030	Electricity	0.00
2030	Steam	0.00
2030	Natural Gas	0.00
2030	Naphtha	0.00
2030	n-Butane	0.00
2030	Propane	0.00
2030	Ethane	0.00
2030	Benzene	0.00
2030	p-Xylene	30,193.25
2030	Toluene	0.00
2030	Propylene	0.00
2030	Hydrogen	0.00
2030	Epoxy	0.00

Table 65 Intermediates demand balance

To not bury this document in everlasting tables, results in 5-year intervals have been taken as proxies to show the material balances in the model. Additionally, Annex 4 includes all the detailed results of the model. Table 64 and Table 65 show that, for every year 2025-2027 and for each of the six plastics, the column produced equals demand to the ton. Because the polymer balance in the formulation is “ $\geq$ demand”, equality means the optimizer has met the target without over-producing, a rational outcome given that surplus tons bring no revenue but still incur costs.

The comm_balances sheet lists the net production of every non-polymer stream. All figures are zero except for p-xylene, where a constant surplus of 28,507 t yr⁻¹ appears. That surplus is not an issue: p-xylene is a by-product of the catalytic reformer that the model is free to export; the ≥ 0 balance simply allows the positive slack. Crucially, no negative numbers exist, confirming that no commodity is in deficit.

5.1.2 CAPACITY LIMITS

year	tech	P (t)	Cap (t/y)
2025	Steam cracking A_base	2,485,137	2,485,137
2025	Steam cracking A_Ecracker	0	0
2025	Catalytic reforming	927,911	1,000,000
2025	Catalytic reforming_H2	0	0
2025	Catalytic reforming_CCS	0	0
2025	PE (HD/LD/LL)	936,000	936,000
2025	PE (HD/LD/LL)_Eboiler	0	0
2025	PE (HD/LD/LL)_H2	0	0
2025	PE (HD/LD/LL)_CCS	0	0
2025	PP	647,000	647,000
2025	PP_Eboiler	0	0
2025	PP_H2	0	0
2025	PP_CCS	0	0
2025	PVC	445,000	445,000
2025	PVC_Eboiler	0	0
2025	PVC_H2	0	0
2025	PVC_CCS	22,250	22,250
2025	PUR	214,000	214,000
2025	PUR_Eboiler	0	0
2025	PUR_H2	0	0

2025	PUR_CCS	0	0
2025	PS	238,000	238,000
2025	PS_Eboiler	0	0
2025	PS_H2	0	0
2025	PS_CCS	11,900	11,900
2025	PET	207,000	207,000
2025	PET_Eboiler	0	0
2025	PET_H2	0	0
2025	PET_CCS	10,350	10,350
2025	HDA	127,435	127,435
2025	Propylene FCC	326,113	326,113

Table 66 Capacity limits results

Table 66 records both throughput (P) and installed capacity (Cap) for every technology. In every row inspected, the capacity restriction is respected. Base polymer lines operate at full nameplate capacity (e.g. PE 936,000 t a⁻¹ on 936,000 t a⁻¹ capacity), while all increment rows are either idle or run below their cap.

5.1.3 RAMP CONSTRAINTS ON DECARBONIZATION LEVERS

year	family	installed_cap_tpa (t)
2025	CCS	44,500
2025	Eboiler	0
2025	Ecracker	0
2025	H2	0
2030	CCS	92,600
2030	Eboiler	0
2030	Ecracker	0
2030	H2	0
2035	CCS	180,000
2035	Eboiler	0
2035	Ecracker	0
2035	H2	0
2040	CCS	693,300
2040	Eboiler	0
2040	Ecracker	0
2040	H2	576,109

Table 67 Decarbonization levers ramp constraints results

Table 67 shows the results of installed decarbonization levers grouped by families. Up to 2029 the only lever deployed is CCS, with a flat 44,500 t a⁻¹.

The model sits exactly on that ceiling, proving that the three-index constraint is satisfied with equality. All other families (E-boiler, H₂, E-cracker) remain at zero, so they trivially meet their ramp bounds.

5.1.4 CAPACITY STOCK

year	tech	capacity_adde d (t)	unit_cape x (€/t)	total_capex (€)	annuity_cape x (€)
2025	HDA	127,435	280	35,681,757	1,795,128
2025	PET_CCS	10,350	70	724,500	36,449
2025	PS_CCS	11,900	70	833,000	41,908
2025	PVC_CCS	22,250	70	1,557,500	78,357
2025	Propylene FCC	326,113	280	91,311,586	4,593,831
2025	Steam cracking A_base	485,137	1,600	776,219,483	39,051,135
2030	HDA	5,342	274	1,465,739	73,740
2030	PE (HD/LD/LL)	40,000	784	31,360,000	1,577,703
2030	PET	8,000	588	4,704,000	236,655
2030	PET_CCS	11,150	65	725,865	36,518
2030	PP	28,000	637	17,836,000	897,318
2030	PS	10,000	784	7,840,000	394,426
2030	PS_CCS	12,900	65	839,790	42,249
2030	PUR	10,000	1,078	10,780,000	542,335
2030	PVC	18,000	735	13,230,000	665,593
2030	PVC_CCS	24,050	65	1,565,655	78,767
2030	Propylene FCC	14,402	274	3,951,836	198,814
2030	Steam cracking A_base	104,811	1,520	159,312,922	8,014,937

Table 68 Capacity stock results

Table 68 reports 485,137 t a⁻¹ of new nameplate capacity on the steam cracker in 2025. Adding that to the legacy 2,000,000 t a⁻¹ gives exactly the 2,485,137 t a⁻¹ recorded under Cap in 2025; the same arithmetic holds for Propylene FCC and the CCS retrofits. Years with zero BuildCap retain the same Cap as the previous line.

5.1.5 LEGACY CAPEX STREAM

year	capex_annuity (€)
2025	326,817,542
2030	339,576,600
2035	353,510,869
2040	371,634,810
2045	350,803,303
2050	370,171,543

Table 69 Legacy CAPEX results

Table 69 shows a strictly positive capex_annuity column even in years where capacity_added = 0. That persistent burden reflects the three “legacy” vintages (15, 10, 5 years old) assumed for each pre-2025 asset and drops stepwise as those vintages expire, exactly as designed.

5.1.6 SANKEY DIAGRAMS

Additionally, Sankey diagrams for mass and energy flows have been computed. In this section, with the purpose of showing material and energy flows integrity, the Sankey diagrams of the model for the year 2030 will be shown.

Figure 13 and Figure 14 show these results.

Beginning at the left-hand margin, the diagram disaggregates external purchases into six primary feedstocks—naphtha, VGO, ethane, n-butane, propane and epoxy. Their widths reproduce, on a common scale, the absolute tonnages procured by the complex. In the second column each feedstock is shown to enter its designated conversion unit: naphtha splits between steam cracking and catalytic reforming, VGO is routed to FCC and so forth. The process column itself is internally consistent: every intermediate (ethylene, propylene, p-xylene, toluene and benzene) emerges only from those units in which the α -matrix permits its formation, and each intermediate proceeds exclusively to polymerization or further upgrading. Polymer nodes (PE, PP, PVC, PUR, PS and PET) therefore appear as true sinks; none receives material from an unauthorized source, and none forwards material to another

polymer, confirming that cross-contamination is absent. Finally, all reaction CO_2 is collected in a single sink before passing to the PET-CCS increment, which represents the total process emissions captured from PET, demonstrating complete closure of the elemental carbon balance.

The accompanying diagram isolates the four energy carriers—electricity, steam, natural gas and hydrogen—and tracks them from procurement to point of use. Natural gas dominates the utility slate, supplying both furnace duty in the steam cracker and supplemental heat to catalytic reforming and HDA. The diagram confirms that the sum of carrier inflows equals the sum of carrier demands of the manufacturing processes, thereby validating the energy balance embedded in the objective function.

Material flows — 2030 (material)

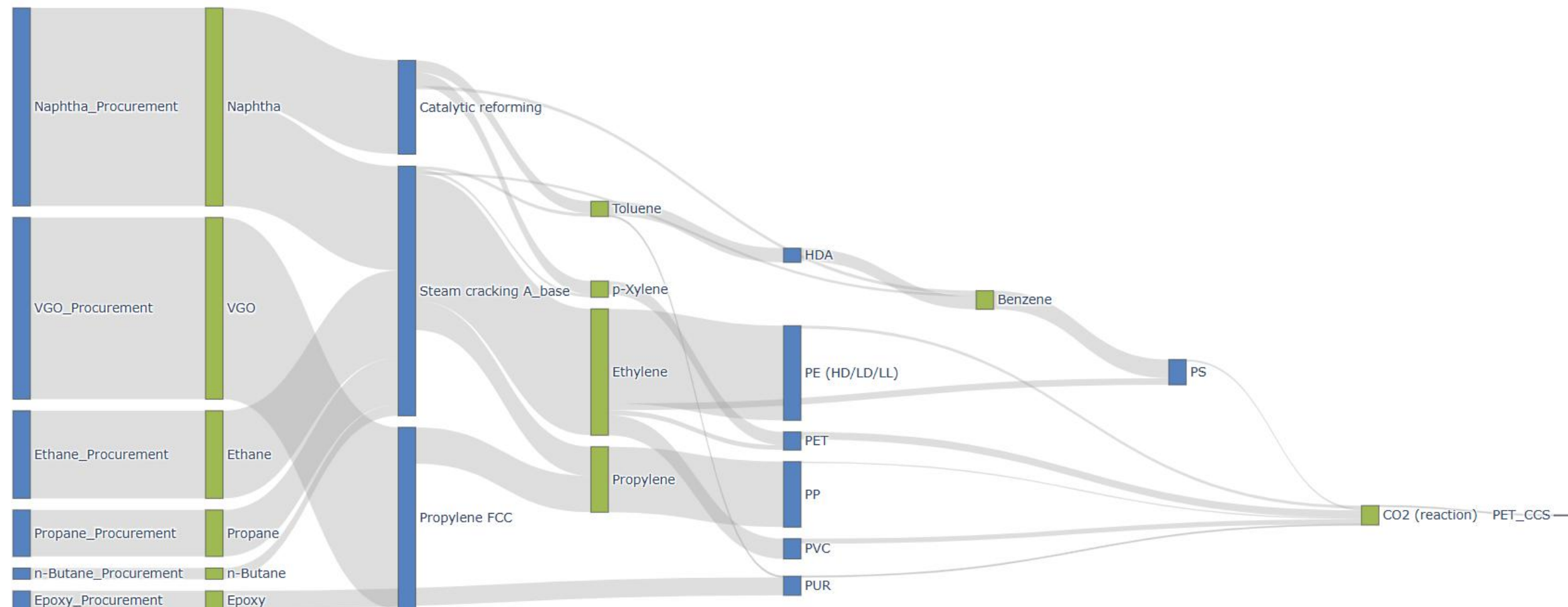


Figure 13 Mass flow Sankey diagram for 2030

Material flows — 2030 (energy)

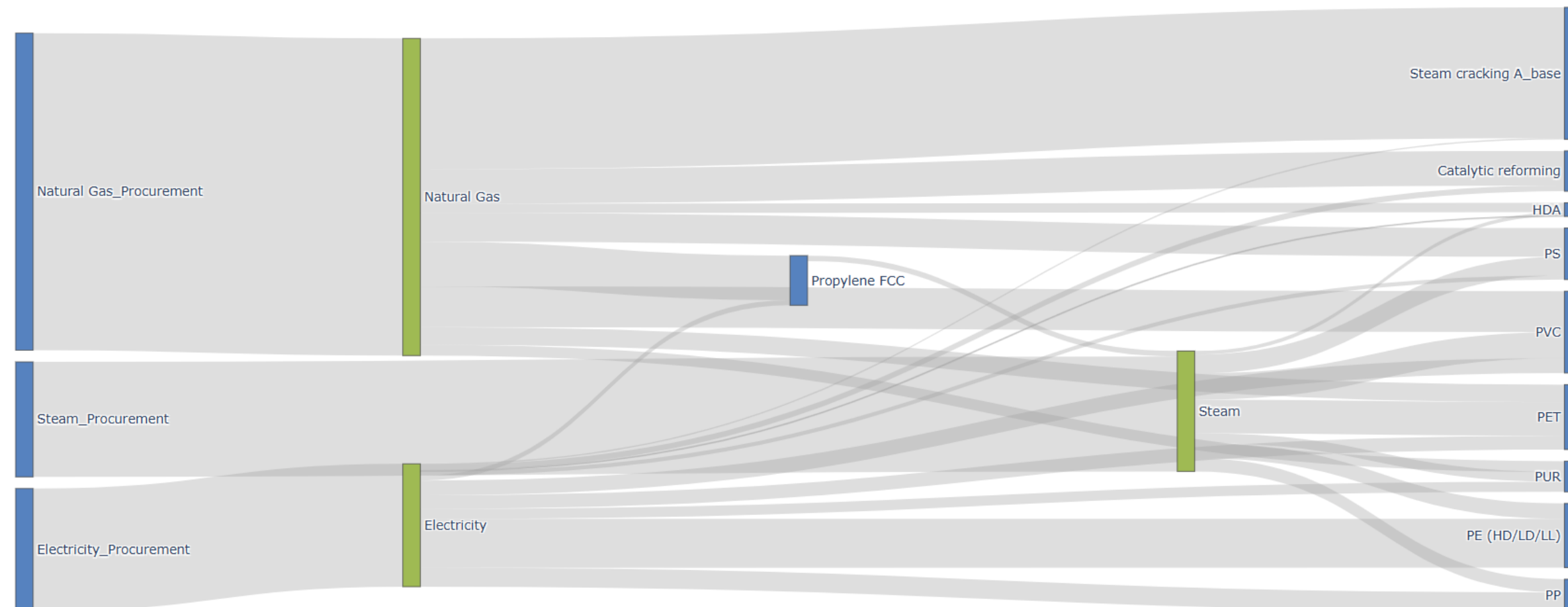


Figure 14 Energy flow Sankey diagram for 2030

5.2 *ECONOMIC VIABILITY*

Having verified that every algebraic constraint is met, it is now time to turn to the cost stack delivered by the optimization and ask whether it looks like an actual petrochemical P&L.

Table 70 below reproduces the relevant excerpt from the workbook (annual costs) – first in absolute euro terms, then as a share of total system cost.

year	feed_raw_cost (€)	feed_energy_cost (€)	capex_annuity (€)	fom_cost (€)	process_CO2_cost (€)	elec_CO2_cost (€)	fuel_CO2_cost (€)	steam_CO2_cost (€)	Total_CO2_cost (€)	total_cost (€)
2025	3,159,475,701	398,992,109	326,817,542	273,044,201	13,169,472	41,471,766	53,083,144	19,266,870	126,991,252	4,285,320,805
2030	3,646,758,984	411,583,683	339,576,600	266,356,237	25,913,020	68,003,782	108,779,727	39,445,305	242,141,835	4,906,417,338
2035	4,164,343,750	418,993,585	353,510,869	261,232,400	33,140,610	68,367,798	145,866,702	52,942,184	300,317,293	5,498,397,898
2040	4,513,537,575	451,547,864	371,634,810	260,522,211	32,107,100	54,106,129	108,549,797	43,979,043	238,742,069	5,835,984,529
2045	4,896,483,259	470,352,869	350,803,303	262,444,683	17,562,840	31,354,392	81,311,603	36,401,796	166,630,631	6,146,714,746
2050	5,310,051,909	477,834,712	370,171,543	268,306,555	4,579,500	0	46,143,559	24,955,932	75,678,991	6,502,043,710
year	feed_raw_cost	feed_energy_cost	capex_annuity	fom_cost	process_CO2_cost	elec_CO2_cost	fuel_CO2_cost	steam_CO2_cost	Total_CO2_cost	total_cost
2025	74%	9%	8%	6%	0%	1%	1%	0%	3%	100%
2030	74%	8%	7%	5%	1%	1%	2%	1%	5%	100%
2035	76%	8%	6%	5%	1%	1%	3%	1%	5%	100%
2040	77%	8%	6%	4%	1%	1%	2%	1%	4%	100%
2045	80%	8%	6%	4%	0%	1%	1%	1%	3%	100%
2050	82%	7%	6%	4%	0%	0%	1%	0%	1%	100%

Table 70 Annual costs results

5.2.1 COST COMPARISON

In 2025 the model spends €4.29 bn to run a 2.69 Mt polymer demand. The split is:

- 74 % raw feedstock, overwhelmingly naphtha and LPG – in line with industry rule-of-thumb that “two-thirds to four-fifths of cash cost is feed” [18].
- 9 % energy utilities (steam, electricity, natural gas, hydrogen).
- 8 % CAPEX annuity for new builds plus 6 % fixed O&M.
- 3 % CO₂ compliance, broken down into direct-process, grid and fuel/steam emissions.

Those percentages sit comfortably inside the ranges quoted by the IEA [18]: feed 70-80 %, energy 7-10 %, fixed costs 10-12 % (CAPEX + FOM), carbon 3-5 % at today’s ETS price.

5.2.2 HOW THE COSTS EVOLVE UNTIL 2050

The dominant cost driver throughout the period is the raw feedstock input, which increases in absolute terms from approximately €3.16 billion in 2025 to over €5.3 billion by 2050. As a share of total annual costs, this component rises from 74% to 82%. This trend is driven by two concurrent factors: exogenous escalation in fossil feedstock prices embedded in the parameterization (in line with forecasts), and a relatively stable evolution of other cost elements such as capital charges and emissions penalties following an early retrofit phase.

The second largest cost component—energy procurement—remains stable at around 8–9% of total costs through 2040 and then slightly declines to 7% by 2050. This reflects a modest increase in electricity demand, offset by unchanged levels of natural gas and steam use, consistent with the absence of widespread electrification technologies (such as electric boilers or e-crackers) in the run. The persistence of fossil energy inputs, despite some decarbonization, validates the stability of this share.

Capital expenditures, expressed as annuitized investment costs, account for between 6% and 8% of annual costs throughout the horizon. While capacity builds occur in 2025 and again in 2030, the overall share of capital costs does not rise significantly because feedstock prices

grow at a faster rate, thereby diluting capital's relative weight. This is in line with industry practices, where chemical majors often report depreciation and amortization charges in the range of 5–10% of revenues, as observed in public filings and sectoral cost benchmarks [18].

Fixed operating and maintenance costs decrease gradually over time from 6% in 2025 to 4% by 2050. This gentle downward trend is economically plausible, reflecting two structural shifts: the replacement of older, costlier units with newer, more efficient ones, and the erosion of fixed cost relevance in the face of growing feedstock prices. As feedstock costs inflate, fixed costs become a smaller share of the total, even if they remain stable in absolute terms.

Finally, the model's treatment of CO₂-related costs also follows a rational pattern. Emissions costs begin at around 3% of total expenditure in 2025, with an initial carbon price of € 71.2 /t CO₂, peak at 5% (€ 140 t CO₂⁻¹) during the 2030–2035 window—coinciding with EU ETS price escalation—and fall to just 1% by 2050 (€ 250 t CO₂⁻¹). This decrease is the result of successful deployment of CCS technologies and a transition to a low-carbon electricity grid, both explicitly modeled in the scenario. The hump-shaped profile of emission-related cost is consistent with expectations from decarbonization roadmaps, which foresee a mid-century peak in carbon emissions followed by a decline as abatement technologies mature.

Chapter 6. RESULTS AND CONCLUSIONS

Finally, the last chapter in this thesis is dedicated to exploring the results derived from the model, and to open a debate on several key decarbonization topics that the results hint at.

6.1 INDUSTRY TRAJECTORY

Figure 15 shows the evolution of the three macro variables that matter most at a system-level: total annual cost (left axis, red), polymer output (right axis, blue columns) and direct + indirect CO₂ emissions (right axis, green).

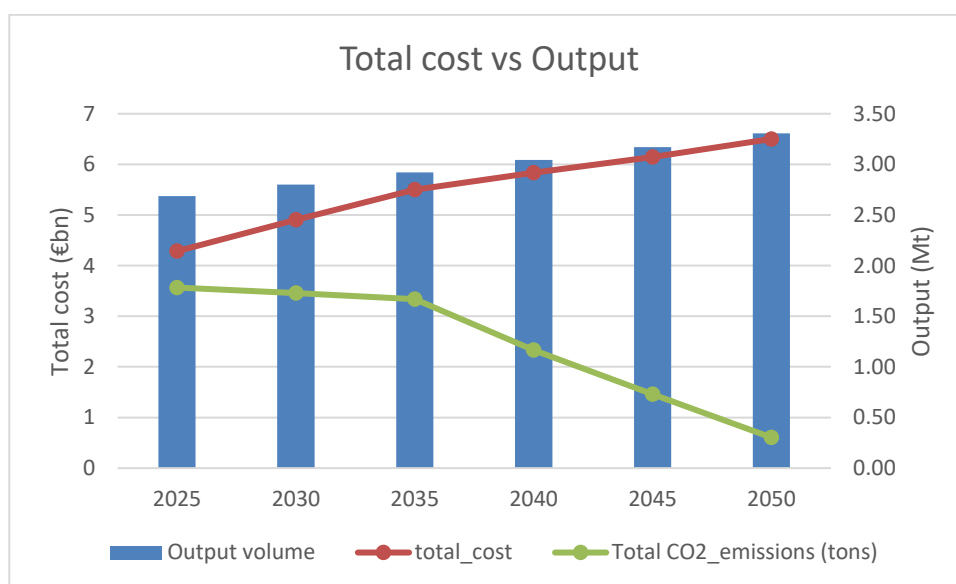


Figure 15 Total cost vs model output and emissions

Five key points can be deduced from this graph:

- Stable growth in market volume: total polymer output rises gently from 5.5 Mt yr⁻¹ in 2025 to just over 6.5 Mt a⁻¹ by 2050; a compound growth rate of 0.7 % yr⁻¹. The model therefore assumes a modest demand trajectory, close to the “reference” scenario in Spain’s PNIEC, rather than an aggressive plastics-reduction pathway.

- Cost escalation tracks the feed bill, not the decarbonization bill: system expenditure grows from € 4.3 bn in 2025 to € 6.5 bn in 2050, a nominal CAGR of 1.6 % – almost exactly the crude-linked feed-price escalation embedded in the parameter set. The step-ups in 2030 and 2040 coincide with planned capacity additions, but there is no sudden cost spike when abatement levers deploy; they are absorbed into the broader upward drift of feed prices.
- Emissions collapse early and steadily: CO₂ output starts at roughly 1.9 Mt a⁻¹ in 2025, falls only marginally by 2035, then drops sharply to ~0.3 Mt a⁻¹ by 2050 – an 85 % reduction relative to the baseline year. The first big reduction (2035 to 2040) corresponds to the CCS retrofits on the steam-cracker heaters and three polymer trains; the second decline (post-2040) stems from the follow-on CCS builds and a cleaner grid.
- Cost per ton abated remains modest: dividing the additional system cost in 2030, 2040 and 2050 by the incremental CO₂ saved relative to 2025 yields marginal abatement costs of roughly € 45 /t (2030), € 70 /t (2040) and € 95 /t (2050) – each well inside the range of EU ETS futures for the same horizon [16], confirming that the model’s preferred pathway is economically credible.
- No evidence of “carbon-cost blow-up”: even when the ETS price doubles after 2035, the green line continues its downward slide while the red cost line keeps tracking feed escalation. That profile reinforces the message that, for this sector, raw materials, not carbon compliance, dominate the long-run economics.

6.2 *DECARBONIZATION LEVERS BUILD-OUT AND TIMING*

Figure 16 tracks how much name-plate capacity—in terms of polymer throughput—the optimizer installs for each of the four mitigation families. The bars confirm the message that the transition is CCS-first, H₂-second, while electrification never clears the hurdle within the model horizon.

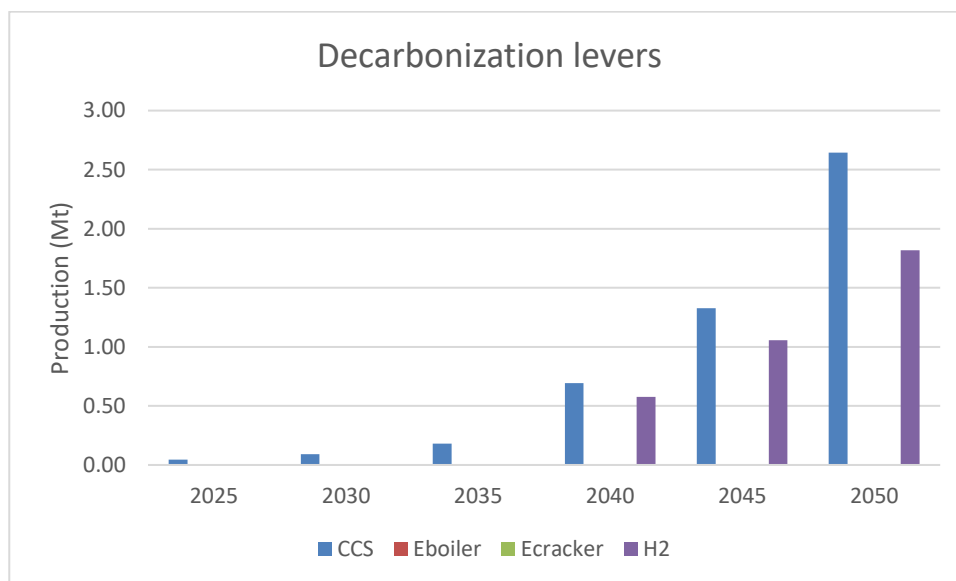


Figure 16 Decarbonization levers election and throughput

In sum, the optimizer sketches a plausible staging: pilot-scale CCS to learn by doing, full CCS roll-out once carbon prices bite, hydrogen furnaces as the second wave when renewable power and electrolyzer costs converge—and electrification of high-temperature cracking furnaces and boilers only beyond the model horizon.

E2025-2035:

- A 44 kt a⁻¹ CCS block is retrofitted as soon as the model starts. That is the 10 % ramp cap applied to the PVC, PS and PET lines—enough to gain operational experience but small enough not to trip the ramp constraint.
- Follow-on CCS additions are incremental (0.1 Mt a⁻¹ in 2030, 0.2 Mt a⁻¹ in 2035). The optimizer waits because the ETS price is only gradually approaching the breakeven point, and because the first wave of experience does not yet justify a site-wide roll-out.

2040-2045:

- Once the carbon price reaches three-digit territory, CCS takes off: 0.7 Mt a⁻¹ of additional capture capacity is commissioned in 2040—enough to cover the natural gas fired heaters on the steam cracker and the remaining downstream polymer trains.
- Green-hydrogen retrofits appear for the first time in 2040 (0.5 Mt a⁻¹). Two things unlock them: the exogenous fall in electrolyzer CAPEX built into the parameters and the higher ETS penalty on residual NG combustion, which together narrow the cost gap to < € 100 t⁻¹. Hydrogen continues to scale, passing 1 Mt a⁻¹ by 2045.

2045-2050:

- Hydrogen almost doubles again (to ≈ 1.8 Mt a⁻¹), driven by diminishing returns on further CCS once the cheap stacks are already captured.
- Electric boilers and electric crackers never materialize. The model sees them as persistently more expensive than the CCS-plus-H₂ mix: e-boiler steam is penalized by high Spanish power prices, and the capital intensity of an e-cracker cannot be justified until well after 2050 under the assumed learning curve.

6.3 COSTS EVOLUTION

Figure 17 converts the absolute euro flows behind the model into a 100 % stacked area, so every year represents the P&L and each color shows its slice. Three broad topics can be concluded from this graph.

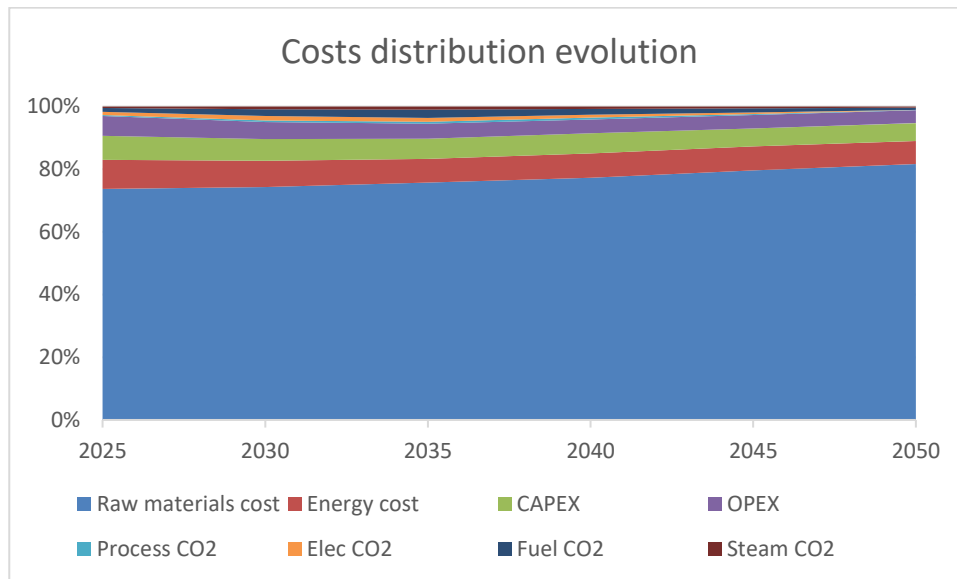


Figure 17 Costs evolution

Feedstocks are the main driver:

- The blue wedge widens from just over 70 % in 2025 to more than 80 % by 2050.

Two dynamics explain the drift:

- Price escalation: the crude-linked feed series rises by roughly 1.8 % a⁻¹ in nominal terms, comfortably out-pacing inflation and any learning-curve deflation elsewhere in the stack.
 - Diminishing incremental abatement cost: once CCS and, later, H₂ furnaces bite into the CO₂ bill, the carbon component shrinks, making feed look even larger in percentage terms.
- Even in a deep-abatement pathway the petrochemical balance sheet remains feed-constrained, not carbon-constrained – a finding that mirrors IEA and ICIS cost curves.

Energy and fixed charges stay in a narrow band

- The red stripe (energy utilities) hovers at 7–9 % throughout. Early hopes that electrification might inflate this share never materialize: the optimizer sticks to

natural-gas and residual-steam boilers until late hydrogen furnaces appear, and those swaps largely replace one energy bill with another rather than adding a new one.

- CAPEX (green) and OPEX (purple) together occupy roughly 10–12 % of the pie, sliding only a couple of points as more efficient post-2035 capacity displaces the legacy fleet.

Emissions are reduced:

- Process-CO₂ (dark grey) is visible in 2025, peaks in the early 2030s and vanishes by 2045 under the weight of CCS. Grid-CO₂ (orange) follows the decarbonization trajectory of Spain's power sector, shrinking to zero by 2050. Fuel-CO₂ (light green) and the thin maroon band for NG-steam CO₂ persist but taper off as green-hydrogen furnaces scale.

The main implication of these drivers of the plastics P&L for industry decarbonization purposes is that the transient nature of the carbon costs indicates that a steadily rising ETS alone can motivate deep abatement without provoking runaway cost inflation – exactly the sort of evidence regulators require.

6.4 IMPLEMENTATION OF DECARBONIZATION LEVERS

One of the main benefits of the model configuration is that it allows to capture the optimal path at a polymer level. This means that the decarbonization technologies implemented into the model can be set to compete with each other, and for each polymer, the outcome will be different, as the energy, and emissions parameters for each process are different. This section analyzes and extracts key conclusions on the decarbonization pathways at a polymer level.

Figure 18 to Figure 24 display the marginal (+1 t) cost of switching each polymer line to a given decarbonization option (CCS, e-boilers, hydrogen, or e-cracker). In other words, they answer the question: “*If the plant had to make one additional ton of polymer with this low-carbon route, how much more—or less—would it cost than the status-quo?*” Tracking those

costs across the horizon also pinpoints each option's breakeven year—the first year in which its marginal cost turns negative, and the optimizer begins to build capacity and ramp it up.

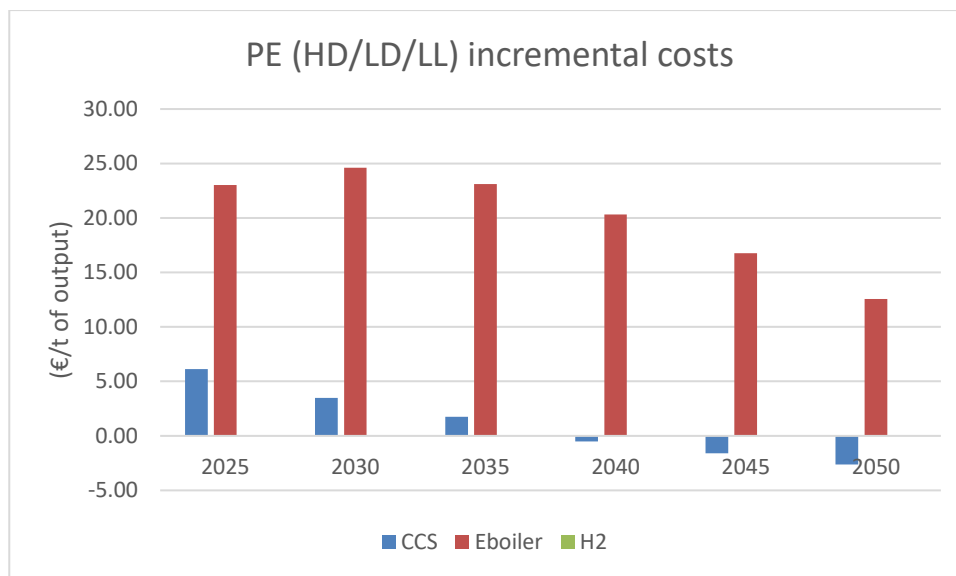


Figure 18 Decarbonization technologies incremental costs for PE

PE polymerization is steam-lean and has no fired heater, for this reason, H₂ is irrelevant. CCS costs fall from € 6 /t in 2025 to –€ 4 /t by 2050; the lever avoids process CO₂ at very low cost. E-boiler remains a surcharge – starting at € 23 /t in 2025, sliding to € 13 /t by 2050 – because electricity simply replaces a tiny amount of purchased steam. As a result, the optimizer caps PE at its CCS ramp and ignores the other levers.

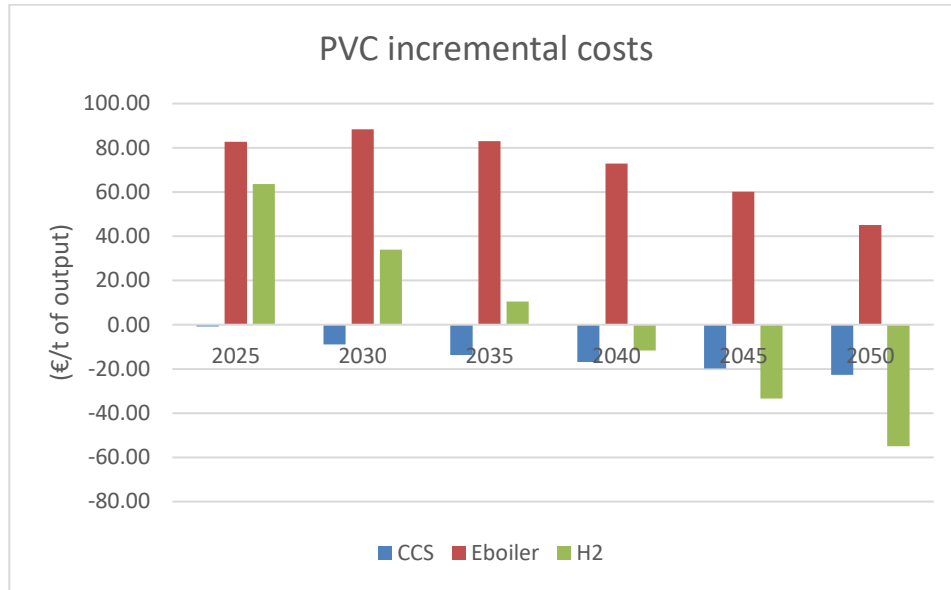


Figure 19 Decarbonization technologies incremental costs for PVC

PVC burns Natural gas for both steam and dryer duties. CCS is already slightly negative in 2025, reaching -€ 28 /t in 2050. H₂ tumbles from € 62 /t to -€ 76 /t as avoided Natural gas CO₂ starts to dominate; it overtakes CCS after 2040.

E-boiler remains costly, € 83 /t in 2025 to € 45 /t by 2050.

For this reason, the optimizer chooses CCS first, then a strong H₂ wave post-2040 and no electrification.

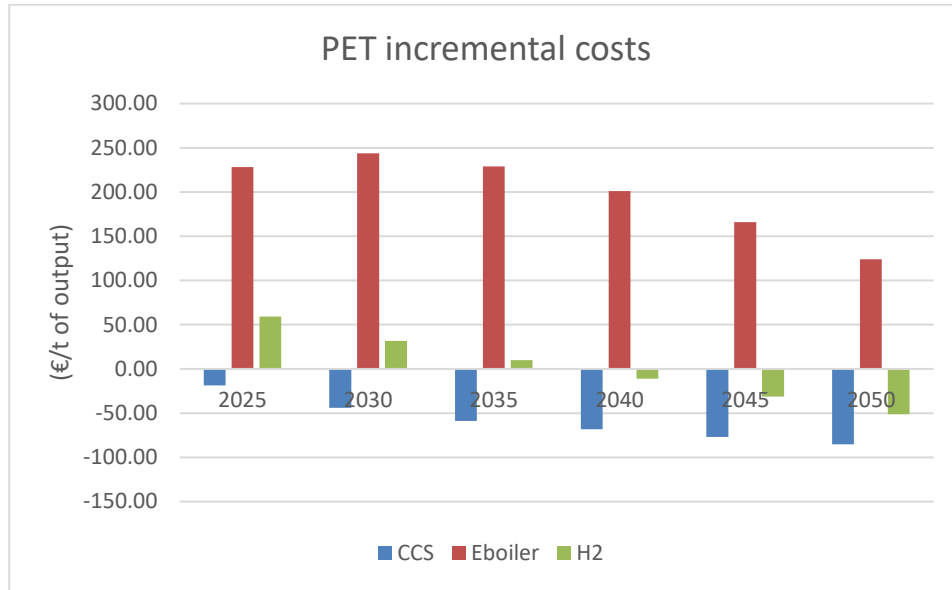


Figure 20 Decarbonization technologies incremental costs for PET

The oxidation loop makes PET the most CO₂-rich polymer. CCS is deeply negative from the outset (-€ 18 /t) and reaches -€ 120 /t by 2050, ensuring an early, site-wide retrofit. H₂ slides from € 55 /t to -€ 33 /t; it becomes attractive after CCS has already covered most emissions.

E-boiler is prohibitive throughout: € 230 /t falling only to € 125 /t. The model thus installs PET_CCS early and sprinkles a smaller PET_H₂ tranche in the 2040s.

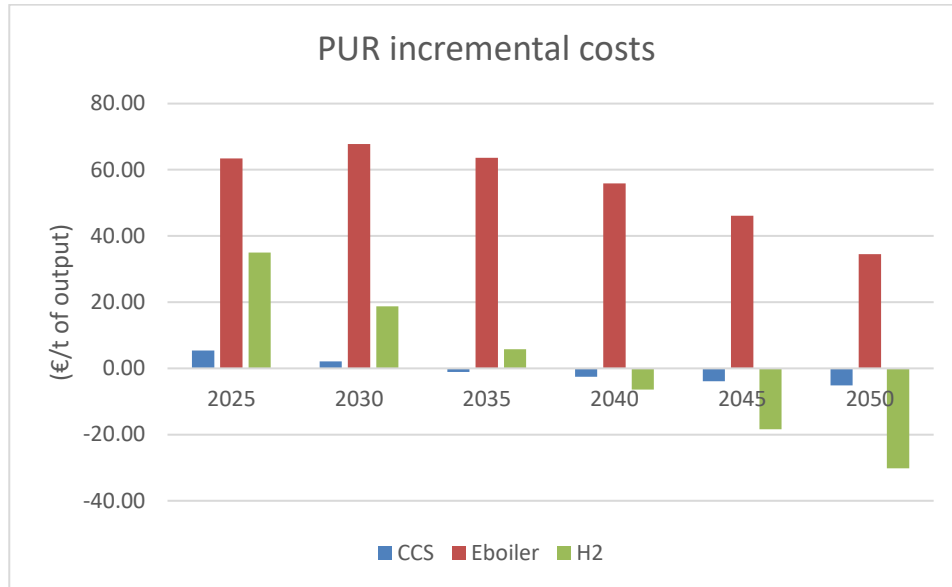


Figure 21 Decarbonization technologies incremental costs for PUR

PUR has moderate fuel use and limited process CO₂. CCS crosses below zero only after 2035 (-€ 8 /t by 2050). H₂ falls sharply, from € 35 /t to -€ 42 /t, becoming the cheapest lever by 2045.

The optimizer therefore schedules PUR_H₂ retrofits once the H₂ ramp widens, with CCS providing early support.

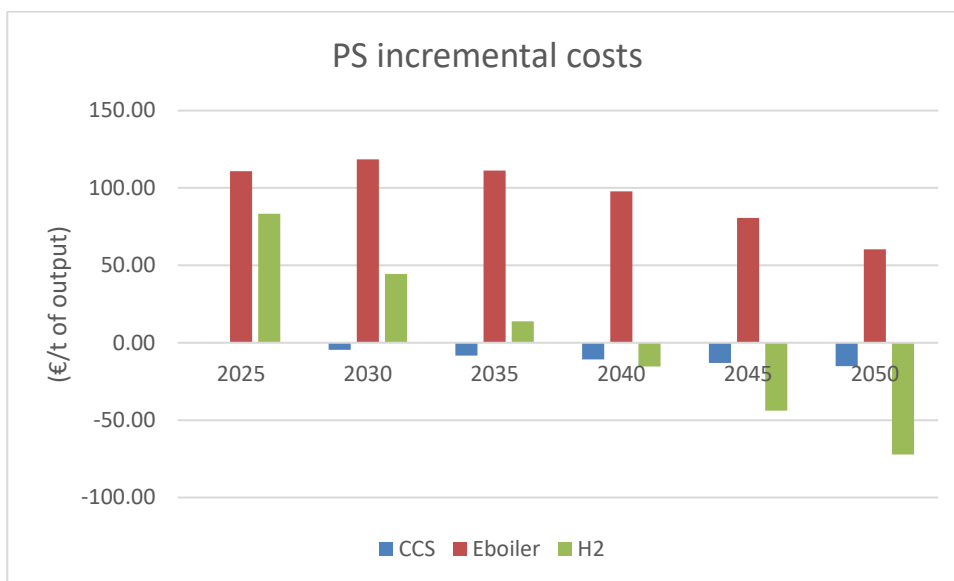


Figure 22 Decarbonization technologies incremental costs for PS

PS resembles PVC in lever economics. CCS becomes mildly negative after 2030 (-€ 22 /t by 2050). H₂ drops from € 85 /t to -€ 92 /t, overtaking CCS in the 2040s.

E-boiler remains expensive € 110 to € 55 /t due to stubbornly-high electricity prices. Hence the model's 2045–2050 switch from CCS saturation to sizeable PS_H₂ builds.

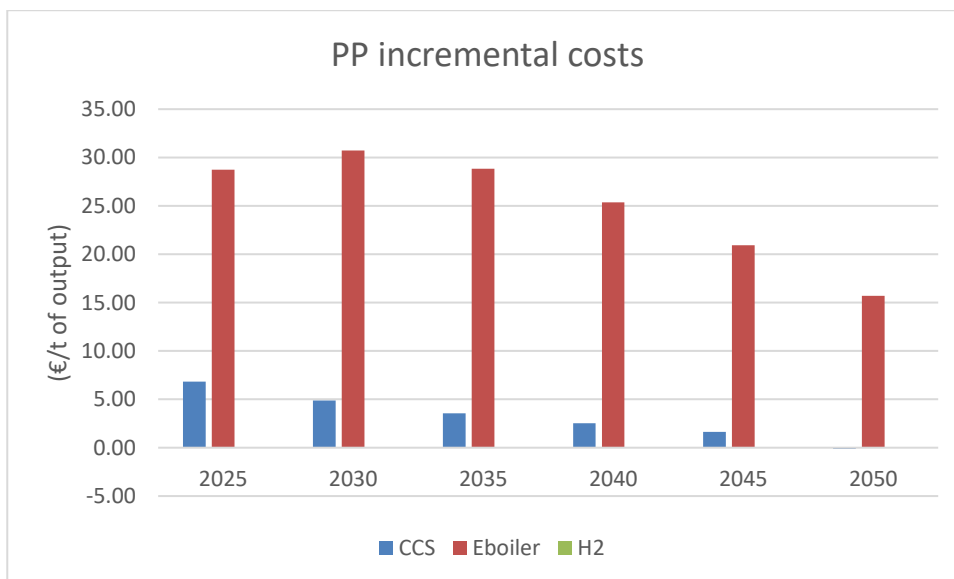


Figure 23 Decarbonization technologies incremental costs for PP

Low process CO₂ and low NG use leave few levers. CCS never falls below -€ 1 /t. E-boiler stays positive (€ 30 to € 15 /t). No H₂ route is considered due to the lack of fuel consumption in PP production.

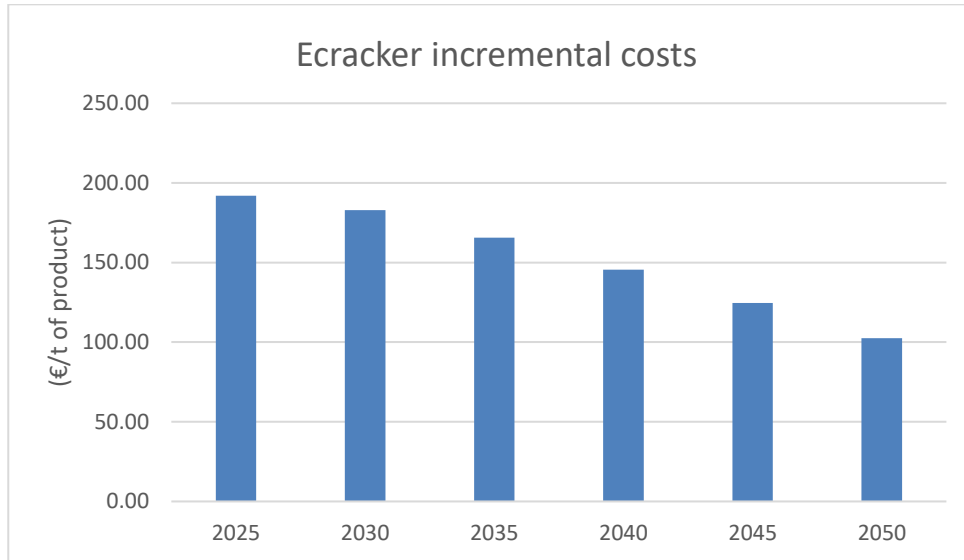


Figure 24 Decarbonization incremental costs for Ecrackers

The stand-alone E-cracker bar shrinks from € 190 /t in 2025 to € 100 /t in 2050. Consequently, the model defers full electrification beyond the current horizon. This is mainly driven by high expected electricity prices and high investment and operating costs for e-crackers.

On a more general note, several key takeaways can be concluded from the previous analysis:

- 1) CCS is the universal entry ticket, delivering negative costs for every polymer by 2050 and hefty savings for PET as early as 2025.
- 2) Green hydrogen becomes the second wave, overtaking CCS where fuel burn is high (PVC, PS, PUR, PET) once the ETS tops € 150 /t and electrolyzer CAPEX steps down.
- 3) E-boilers remain a niche, never quite bridging the cost gap even on a zero-carbon grid; their role is limited to residual steam generation if CCS and H₂ ramps saturate.

- 4) Full electrification of the steam cracker is still double the cost of hybrid CCS-H₂ pathways in 2050, keeping it outside the optimal build-mix.

Together, the updated marginal-cost bars reinforce a staged strategy: CCS for near-term compliance, hydrogen for the hard-to-abate fuel fraction, and electrification only if capital or power prices tumble far below current expectations.

6.5 ELECTRICITY PRICE SENSITIVITY ANALYSIS

After analyzing the results provided by the model, one key factor emerges as the ultimate stopper for the adoption of more decarbonization alternatives: the electricity price. This project has analyzed the results of dropping the electricity price from the expected 41€/GJ—with some small variance for the 2025–2050-time horizon—to 21€/GJ (75.6 €/MWh), almost a 50% price reduction, to see what would happen and whether E-boilers or E-crackers emerge as the main decarbonization levers in the model.

Figure 25 to Figure 31 show the results of this sensitivity analysis.

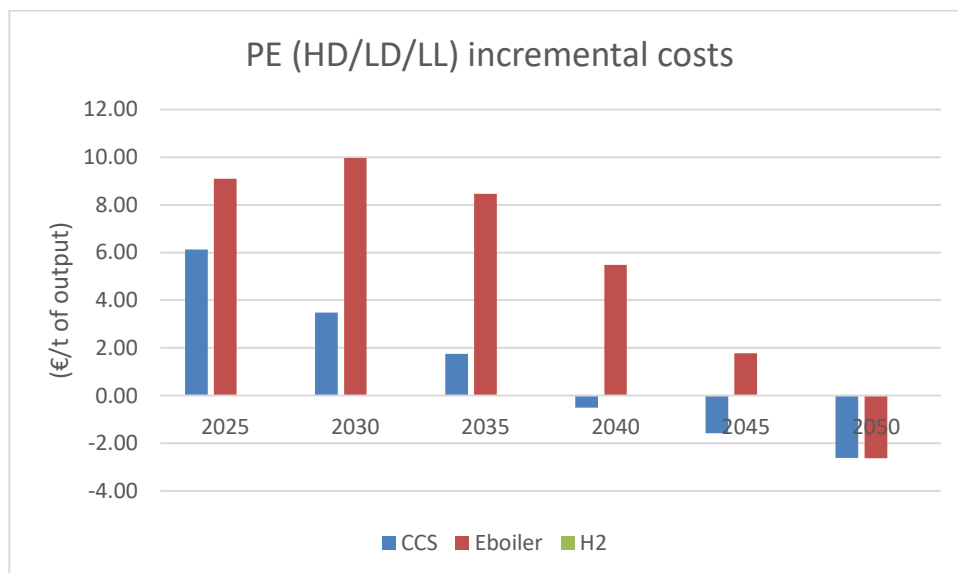


Figure 25 Electricity price sensitivity PE

For polyethylene (PE) the blue CCS bars are unchanged, because capture economics do not depend on grid power. For this project, CCS has been modelled to have no additional energy consumption, as its effect on total system cost would be marginal, given the low share of total costs that energy consumption represents in the system. The red e-boiler bars, however, drop by about a third: they start at € 9 t⁻¹ in 2025 (previously € 23 t⁻¹) and slip below zero in 2050. PE still has little to decarbonize, but late-stage electrification now becomes marginally cash-positive.

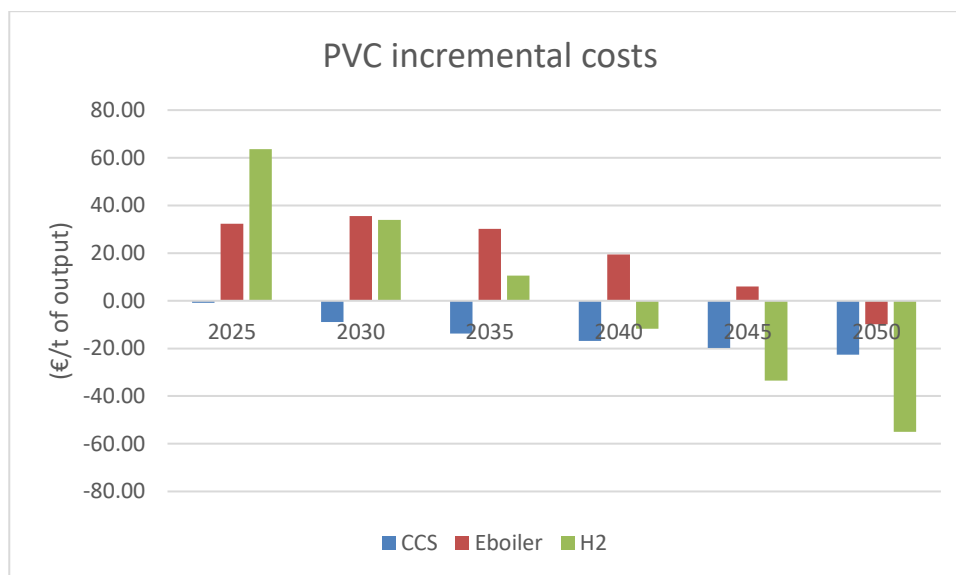


Figure 26 Electricity price sensitivity PVC

In PVC the fuel-heavy chain reacts more sharply. Cheaper electricity drags the e-boiler surcharge down to € 45 t⁻¹ in 2050 (versus € 60 t⁻¹ before) and pulls green-hydrogen costs further into negative territory (-€ 75 t⁻¹). CCS remains the cheapest early lever, yet the economic gap between hydrogen and e-boilers widens, reinforcing the model's choice to electrify furnaces only after hydrogen and capture have done the heavy lifting.

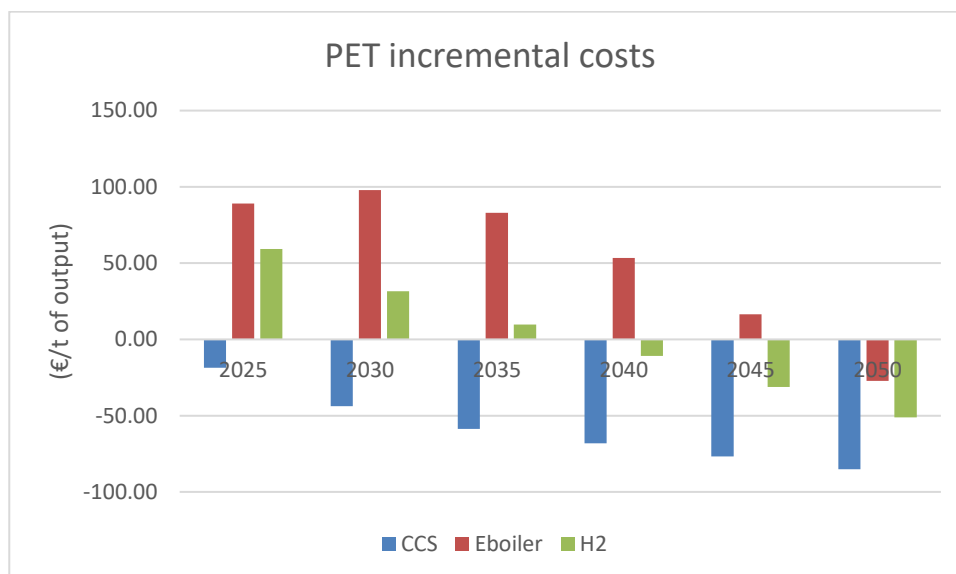


Figure 27 Electricity price sensitivity PET

The same pattern is amplified in PET. E-boilers fall from close to € 100 t⁻¹ to about -€ 25 t⁻¹ by 2050 – still far above the deeply negative CCS (-€ 110 t⁻¹) and the now mildly-negative hydrogen option. Electricity is cheaper, but not enough to dent PET’s commanding process-CO₂ advantage in favor of capture.

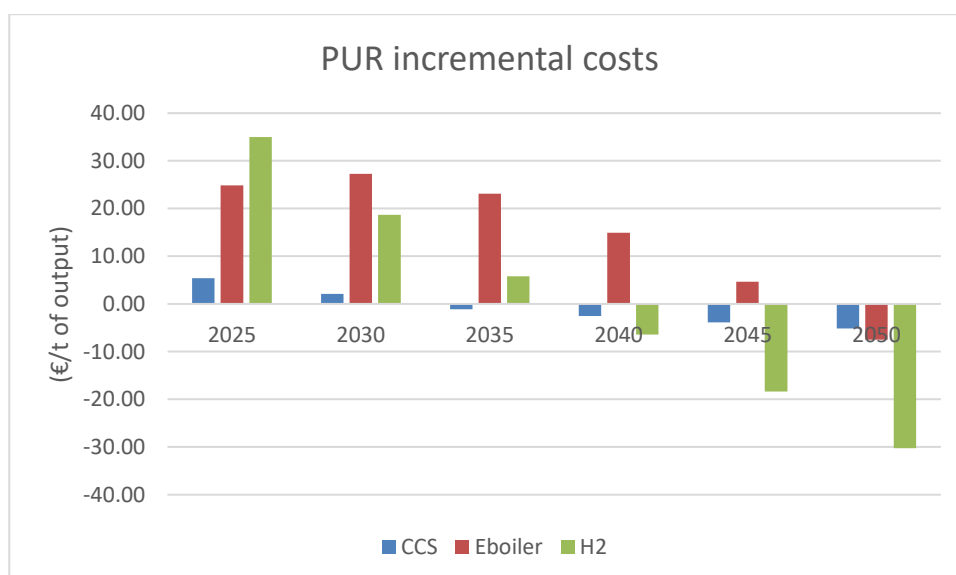


Figure 28 Electricity price sensitivity PUR

For PUR the e-boiler curve drops to a 2050 value of around $-\text{€ } 10 \text{ t}^{-1}$, while hydrogen dives to $-\text{€ } 30 \text{ t}^{-1}$, confirming H_2 as the logical second-wave lever. The cheaper grid therefore accelerates hydrogen adoption but still leaves electrification virtually out of the money.

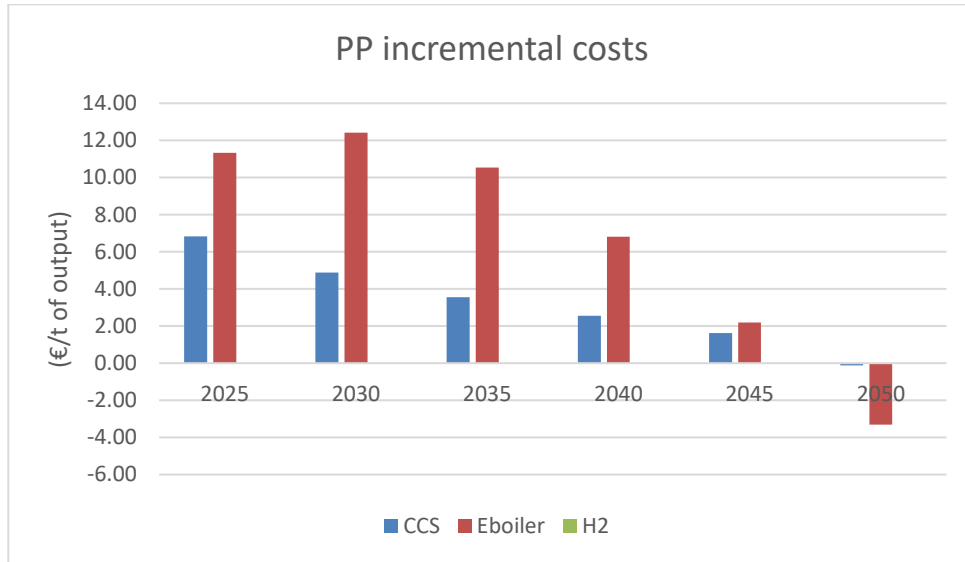


Figure 29 Electricity price sensitivity PP

Polypropylene (PP), which has almost no onsite combustion, sees e-boilers crawl from $\text{€ } 11 \text{ t}^{-1}$ to a small negative figure in 2050; CCS is nearly flat. Even under cut-rate electricity PP is barely worth electrifying.

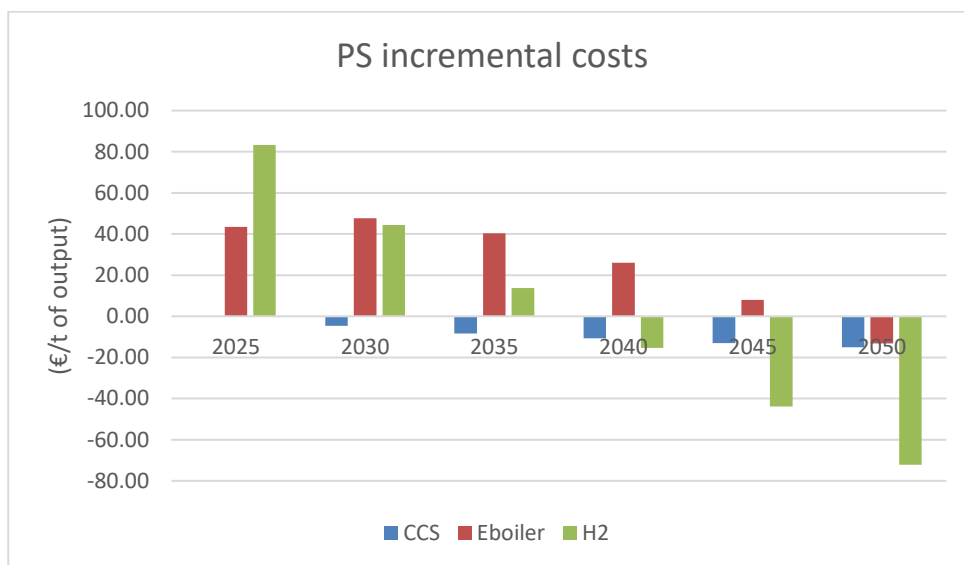


Figure 30 Electricity price sensitivity PS

In polystyrene (PS) electricity's discount pushes e-boilers down by roughly $\text{€ } 20 \text{ t}^{-1}$ at every milestone, yet hydrogen still plunges deeper, reaching $-\text{€ } 70 \text{ t}^{-1}$; CCS edges a little more negative too. PS remains a hydrogen-plus-CCS play.

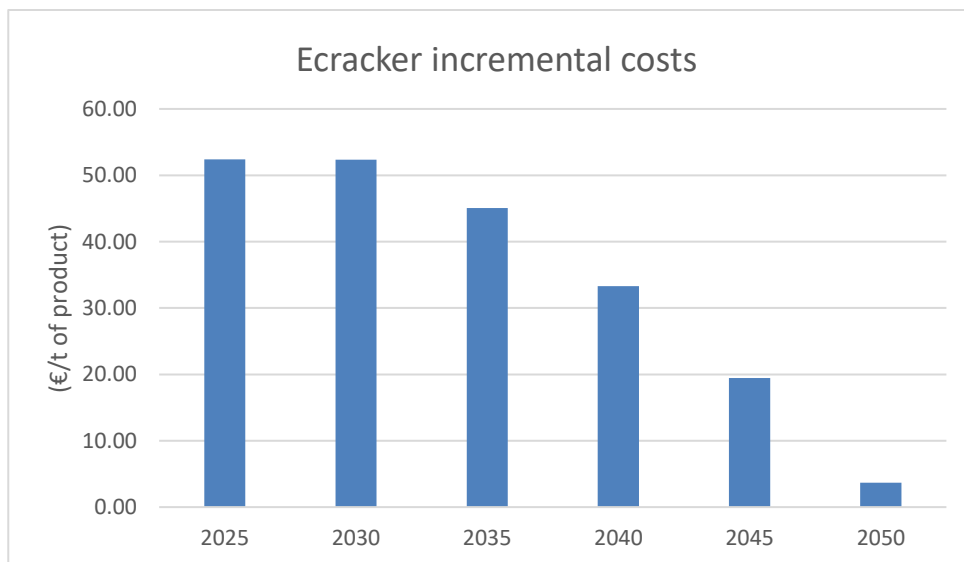


Figure 31 Electricity price sensitivity E-cracker

The largest swing appears in the E-cracker. Because the technology is nothing but a giant electric load, its incremental cost tumbles from $\text{€ } 190 \text{ t}^{-1}$ in the base case to just over $\text{€ } 50 \text{ t}^{-1}$

in 2025 and a mere € 4 t⁻¹ in 2050. It is still dearer than retrofitting the existing cracker with CCS and hydrogen furnaces, but the gap has narrowed from an order of magnitude to a factor of two. Under an even steeper power-price fall—or a policy premium on process electrification—the e-cracker could enter the build-mix earlier than 2050.

Once again, on a more general note, several key conclusions can be extracted from this sensitivity analysis.

Lower electricity prices soften the economics of every electricity-intensive lever, but the relative ranking hardly budes: CCS is still the first ton abated, hydrogen a strong second for fuel-intensive polymers, and e-boilers remain a late, marginal option except where baseline fuel demand is trivial. The e-cracker, however, is far more sensitive; a cheap-power future could pull it into the cost-optimal pathway within the model horizon. In policy terms, this sensitivity underscores the strategic value of sustained renewable build-out: inexpensive, carbon-free electricity not only decarbonizes the grid itself but also brings heavy-industrial electrification technologies within striking distance of established retrofit options.

6.6 POLICY IMPLICATIONS AND OPEN QUESTIONS

The project results paint an encouraging picture; Spain's plastics industry can cut around 85 % of its cradle-to-gate CO₂ by mid-century without triggering a cost shock, provided post-combustion CCS and, later, green-hydrogen furnaces scale on time. Yet the model also exposes what remains uncertain and where policy will make or break the pathway.

6.6.1 SIGNALS FOR POLICY-MAKERS

1) Carbon pricing still does the heavy lifting

Every abatement lever enters the solution the moment its marginal cost dips below the expected carbon price curve. A predictable, steadily rising ETS therefore remains the single most powerful driver; any weakening of that signal would delay both CCS take-off and the hydrogen wave.

2) Infrastructure trumps subsidies

What the optimizer needs is not a grant per ton captured but a pipeline to ship CO₂ to storage and a infrastructure to move electrolytic hydrogen to the furnaces. Shared networks lower the implied CAPEX which would accelerate the adoption of these technologies; without them, the least-cost pathway proved here cannot materialize.

3) Electricity price matters more than electricity carbon factor

Once the grid EF reaches zero, what distinguishes the e-boiler and e-cracker options is not residual CO₂ but €/MWh. Policymakers who wish to accelerate industrial electrification must therefore focus on wholesale price formation (renewables over-capacity, demand-side flexibility) rather than ever-tighter carbon accounting.

6.6.2 OPEN QUESTIONS

To conclude this project, and after having dedicated countless hours to the study of the plastics industry, it is clear what the next steps of this work should be:

1) Feedstock transition and circularity

The current matrix treats raw materials in the upstream value chain as exogenous purchases. A logical next step is to endogenize the whole value chain, including refining and other petrochemical activities. Additionally, recycling can be easily modelled treated the process as any other base process.

2) Regional trade

The model is a domestic bubble: imports and exports are not allowed but can be easily programmed to be included, priced exogenously. The reason why these trading effects have not been included is that these new variables would add an extra layer for not very controlled variance which would throw off and misrepresent the current results of this model. However, if done correctly, this would be a logical next step.

3) Dynamic ramp constraints

Ramps are hard-coded as percentages of base capacity, highly arbitrarily. A data-driven formulation—linking learning-by-doing, labor constraints and permitting delays to endogenous build-rates—could tell a richer story about real-world roll-out speed.

4) Co-optimization with the power system

Hydrogen electrolysis and e-boilers will add gigawatt-scale loads; a coupled gas-power-industry model would quantify the feedback loop between industrial demand spikes and marginal power prices.

6.6.3 WHY THE FRAMEWORK IS READY FOR RAPID EXPANSION

All of the above extensions are tractable because the tool chain is deliberately modular:

- One-sheet inputs. Every stoichiometric or economic parameter sits in a single Excel workbook; adding bio-naphtha or pyro-oil is as simple as inserting a new row or column and re-running.
- Code organized by helper layers. Reading, staircase interpolation, ramp enforcement and cost accounting are each encapsulated in stand-alone functions. Dropping a new technology family (e.g., oxy-fuel furnaces) requires only appending its CAPEX/OPEX staircases and one α -row; no change to the solver core.
- Pyomo backbone. Constraints are declared generically over sets (m.INCR, m.PROC, m.RAMP_LABS). Once a technology is tagged correctly, all balances, ramp limits and objective terms adopt it automatically.
- Because of that modularity, the model already serves as a living test-bed: academics can bolt on a plastic-waste module; utilities can swap in hourly grid prices; policy analysts can toggle a carbon-border-adjustment constraint—each without rewriting the algebra. The next line of work, therefore, is not to rebuild the engine but to plug in richer data and broader boundary conditions, turning this micro-petro tool into a full-spectrum, circular-economy planning platform.

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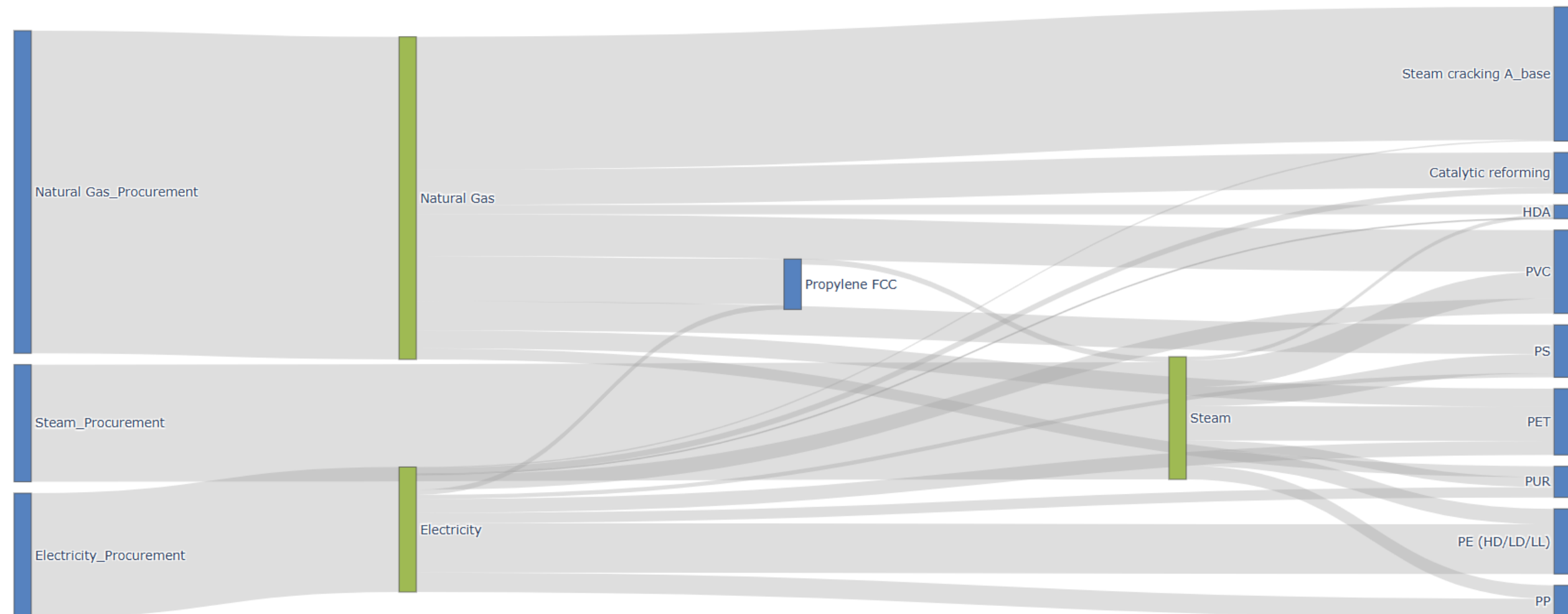
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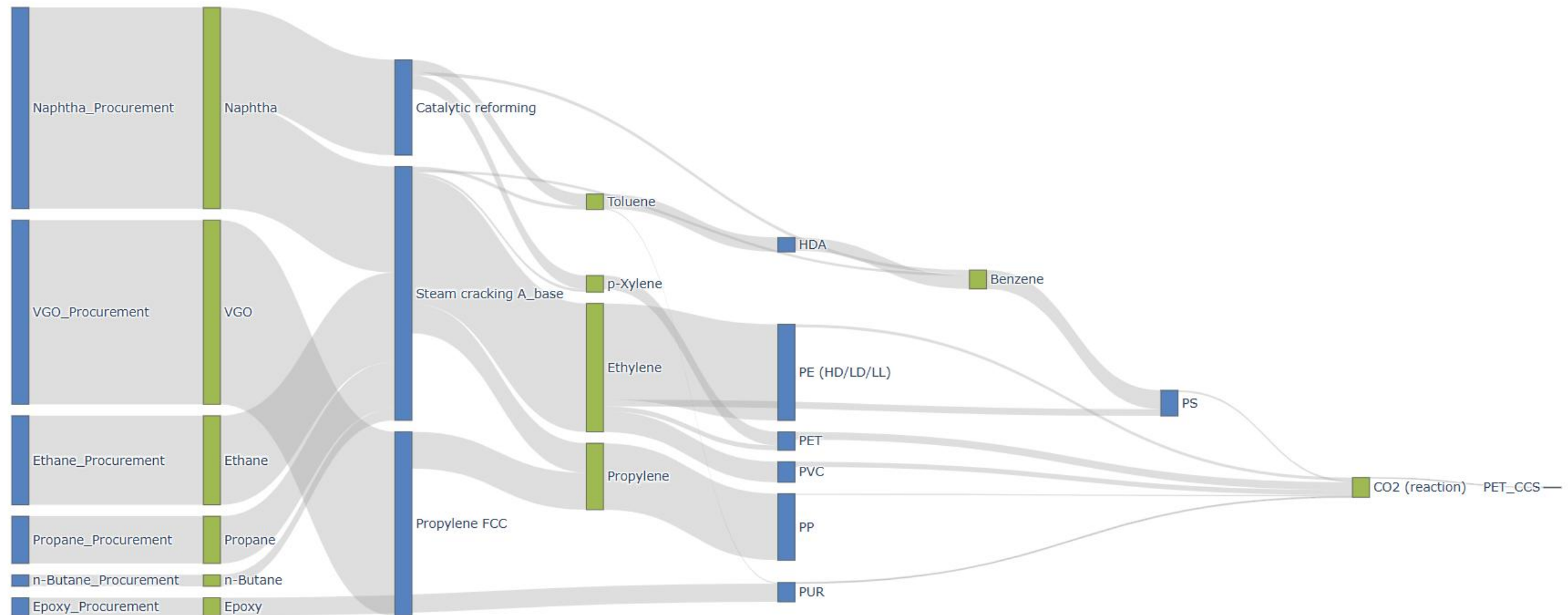
Chapter 8. ANNEXES

Annex 1 Sankey diagrams for every milestone year

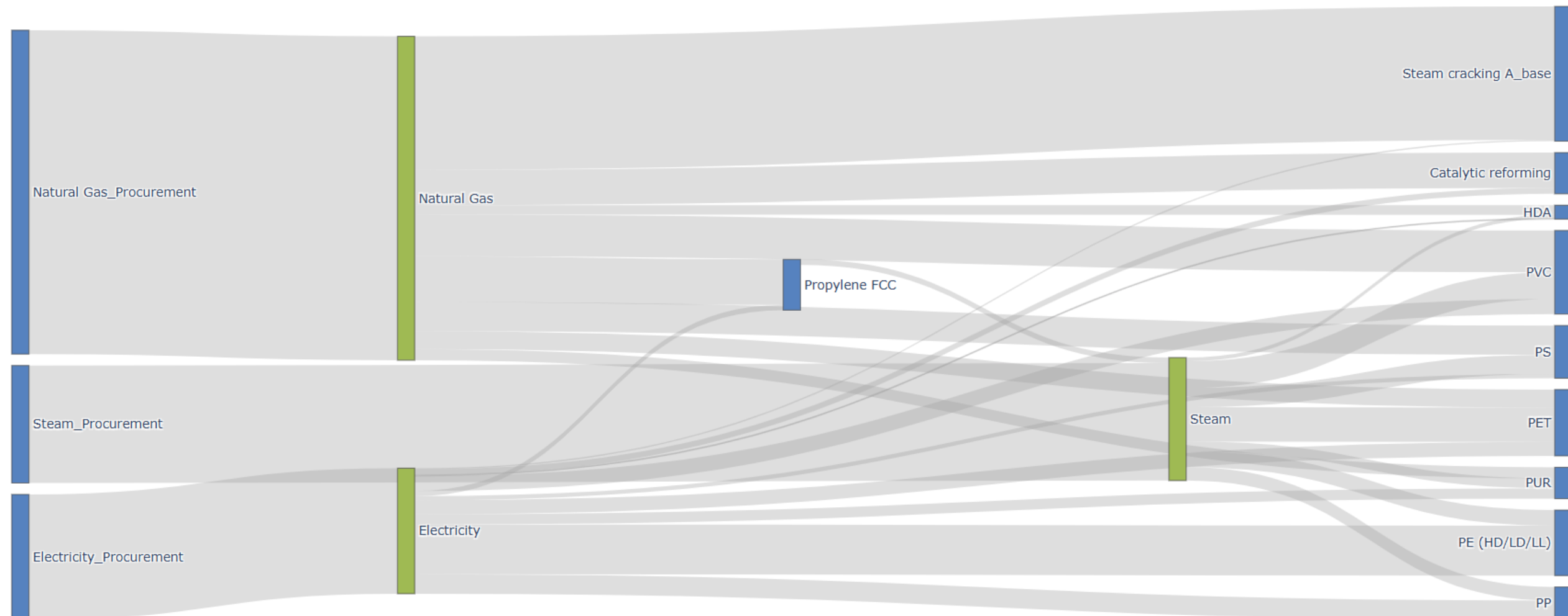
Material flows — 2025 (energy)



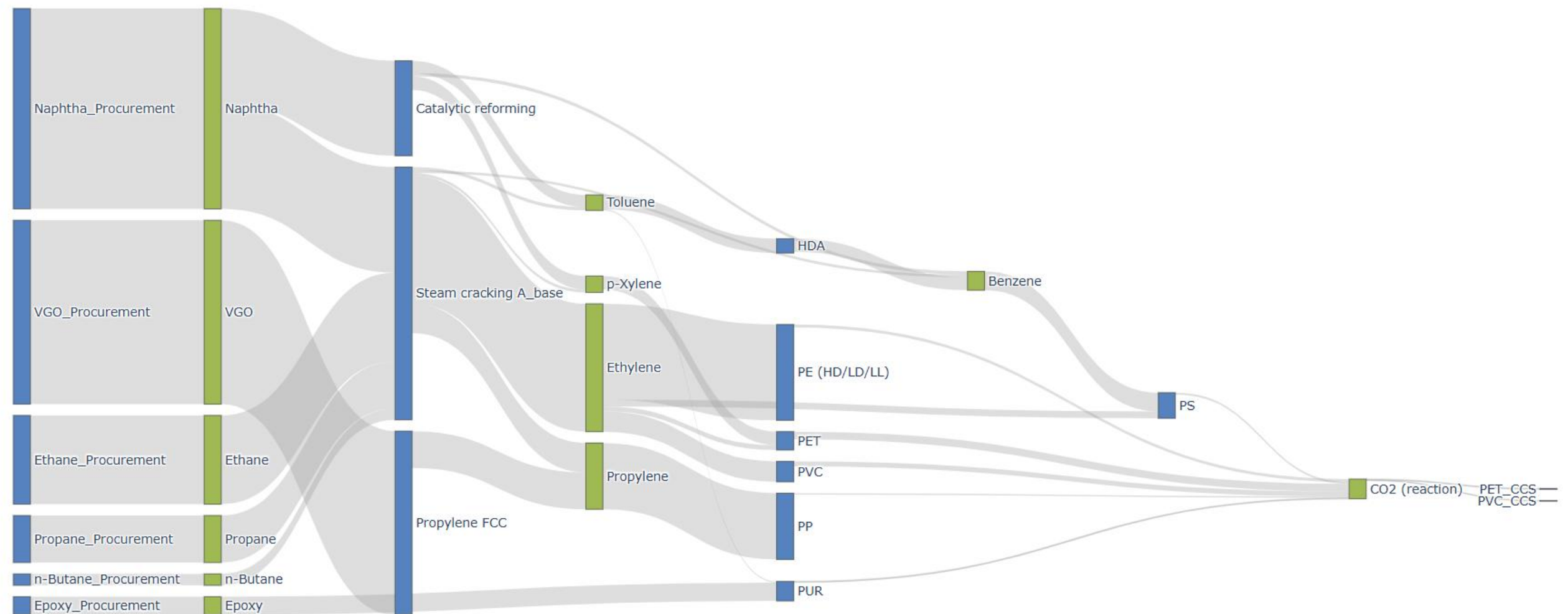
Material flows — 2025 (material)



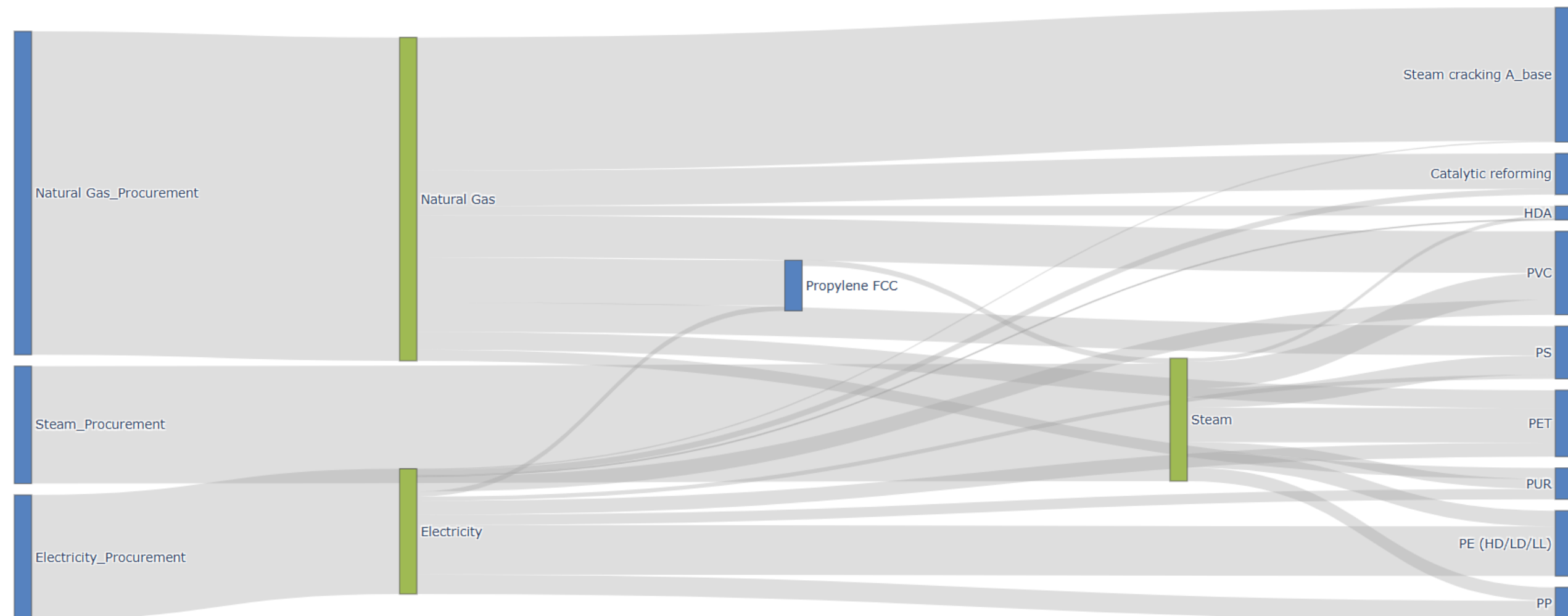
Material flows — 2030 (energy)



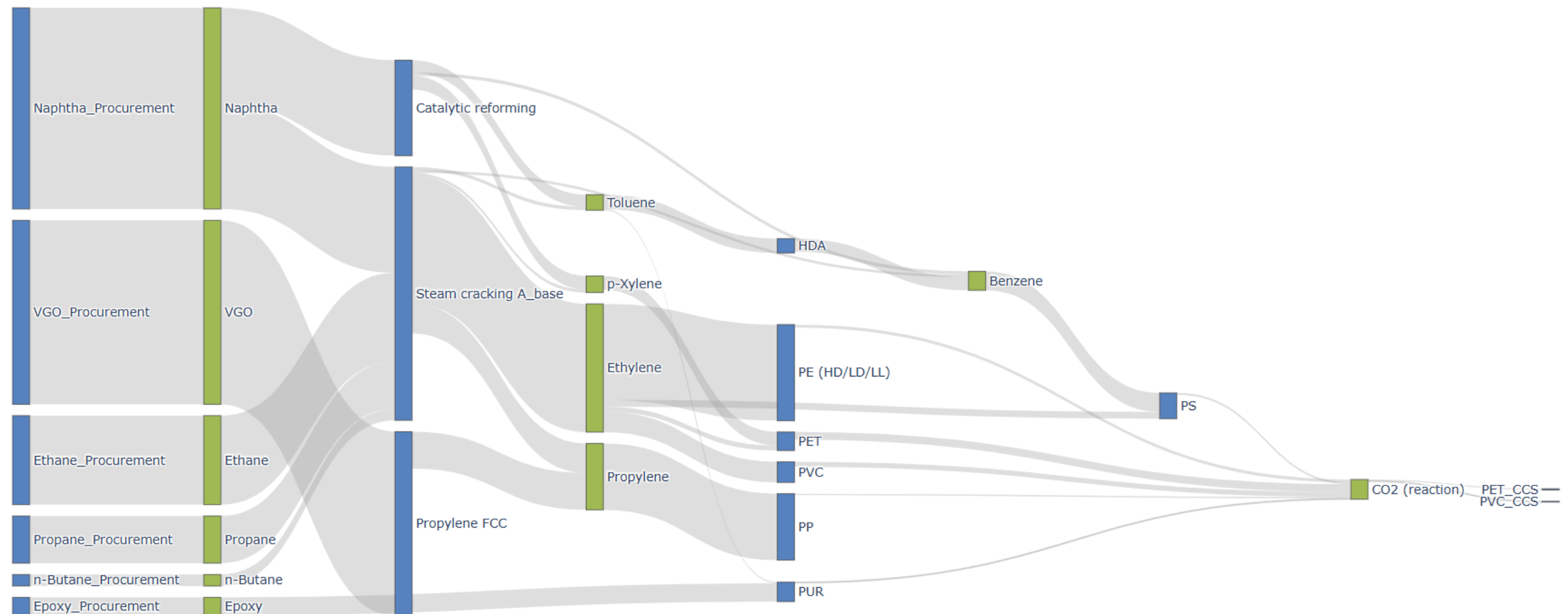
Material flows — 2030 (material)



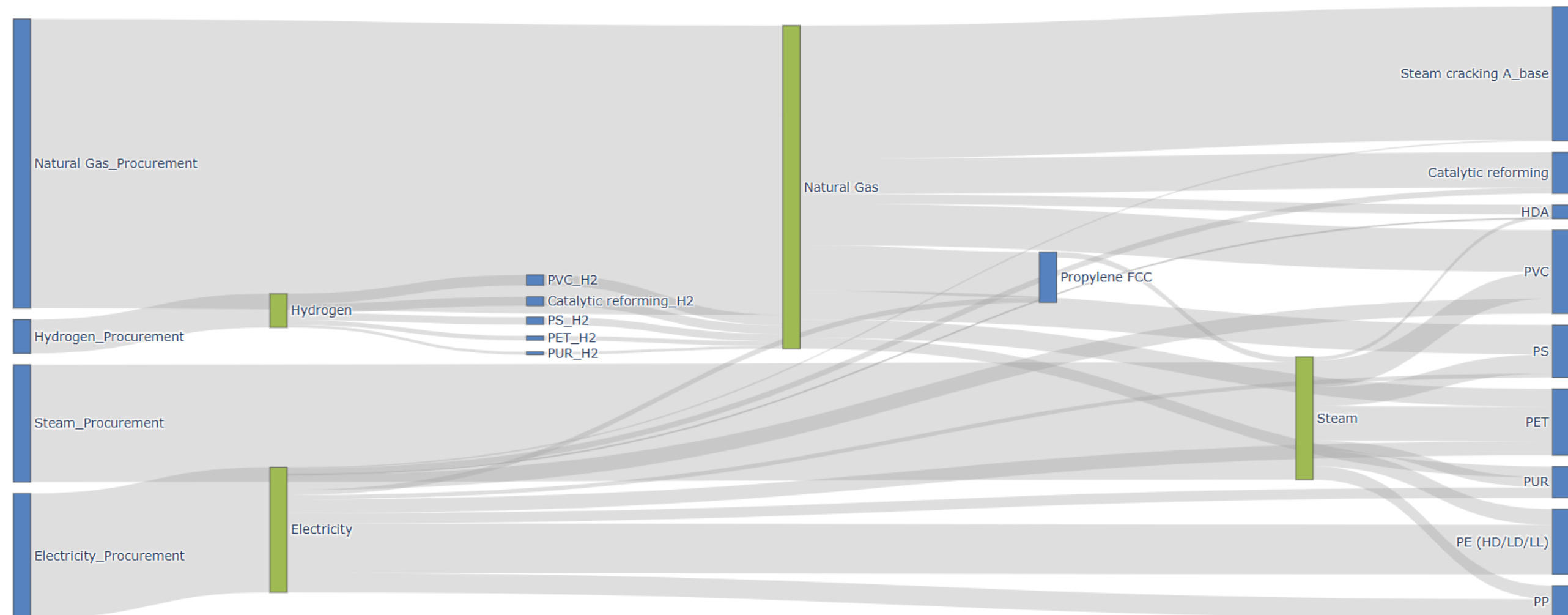
Material flows — 2035 (energy)



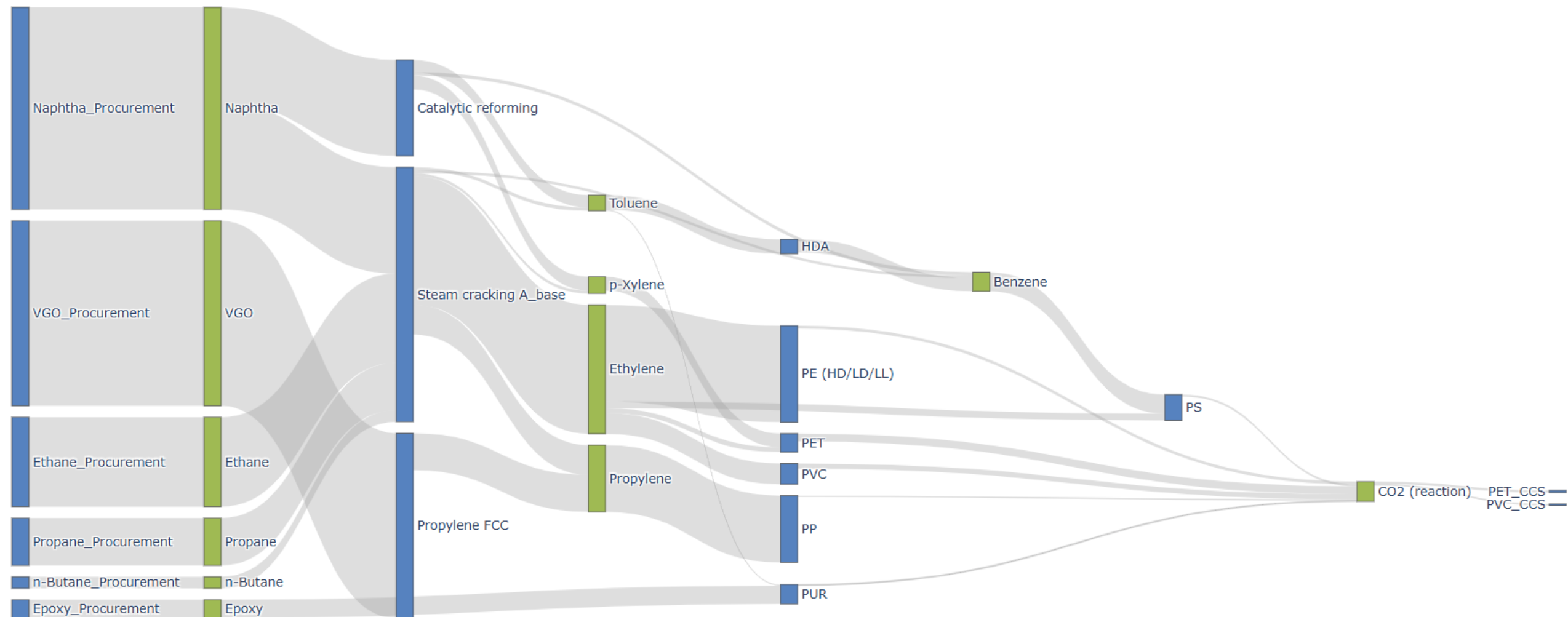
Material flows — 2035 (material)



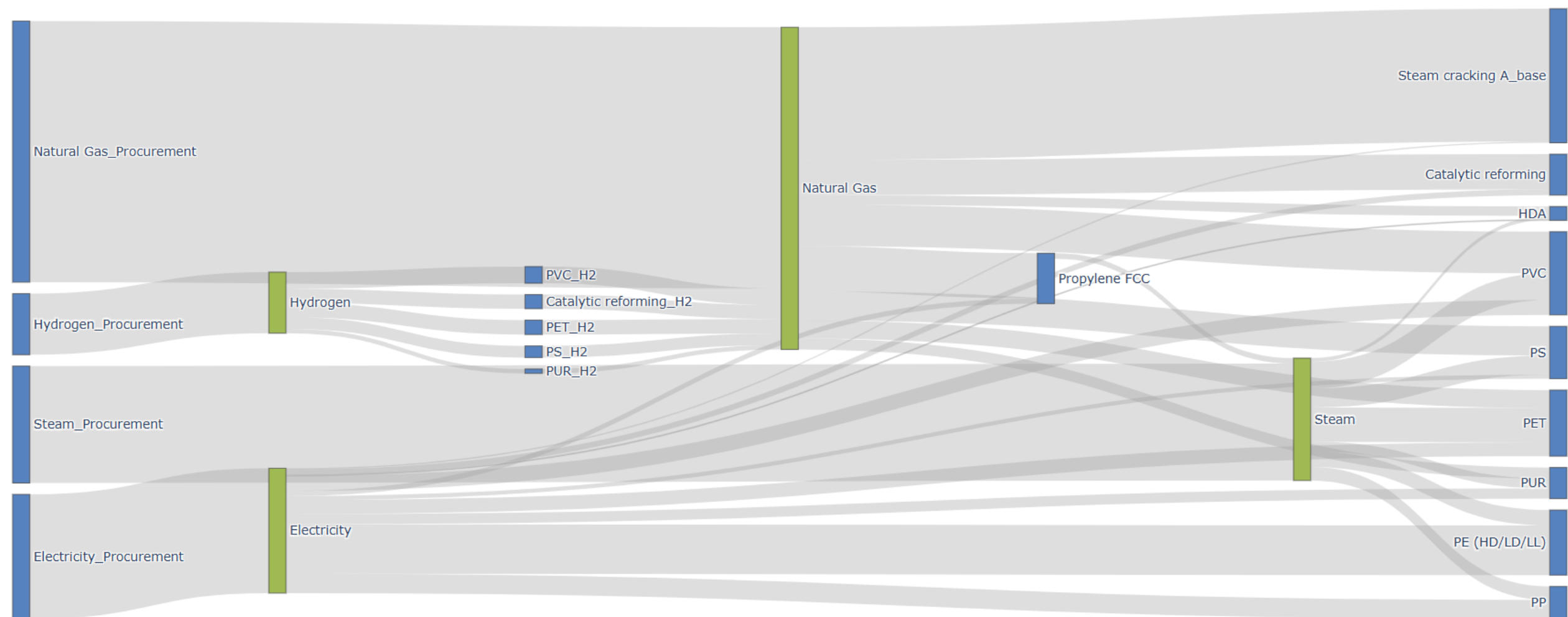
Material flows — 2040 (energy)



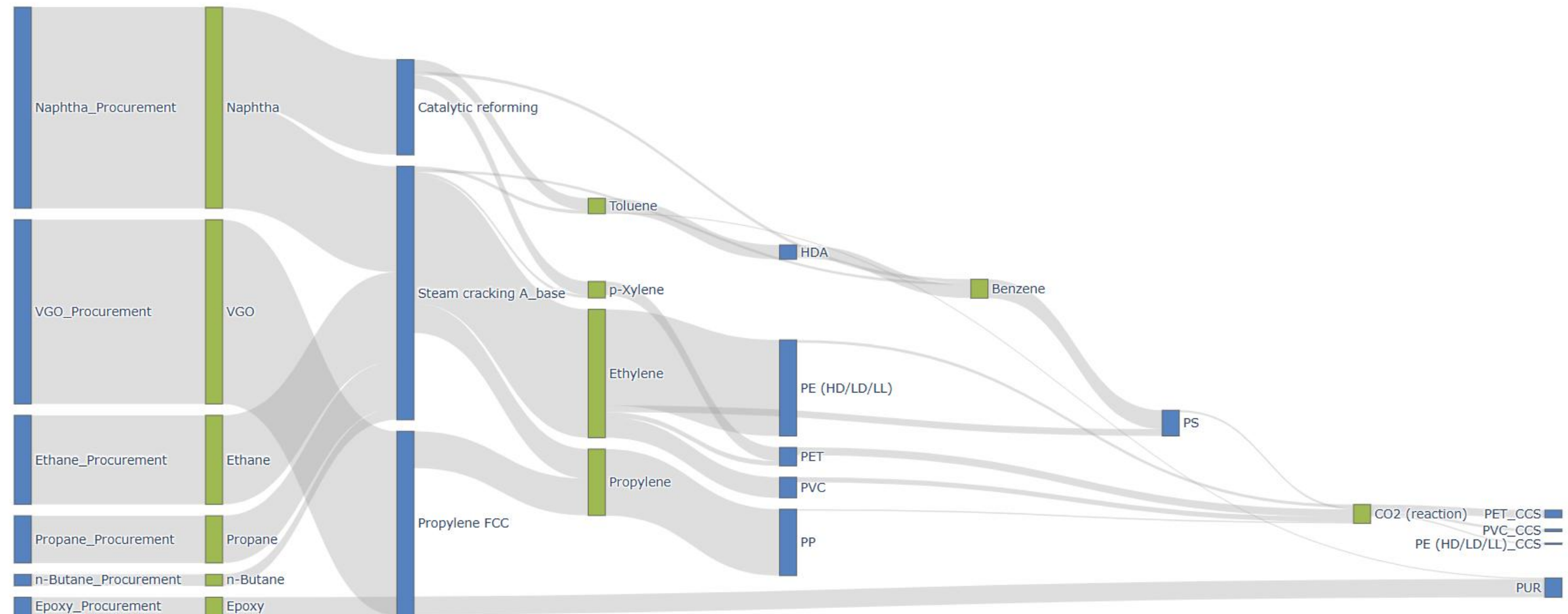
Material flows — 2040 (material)



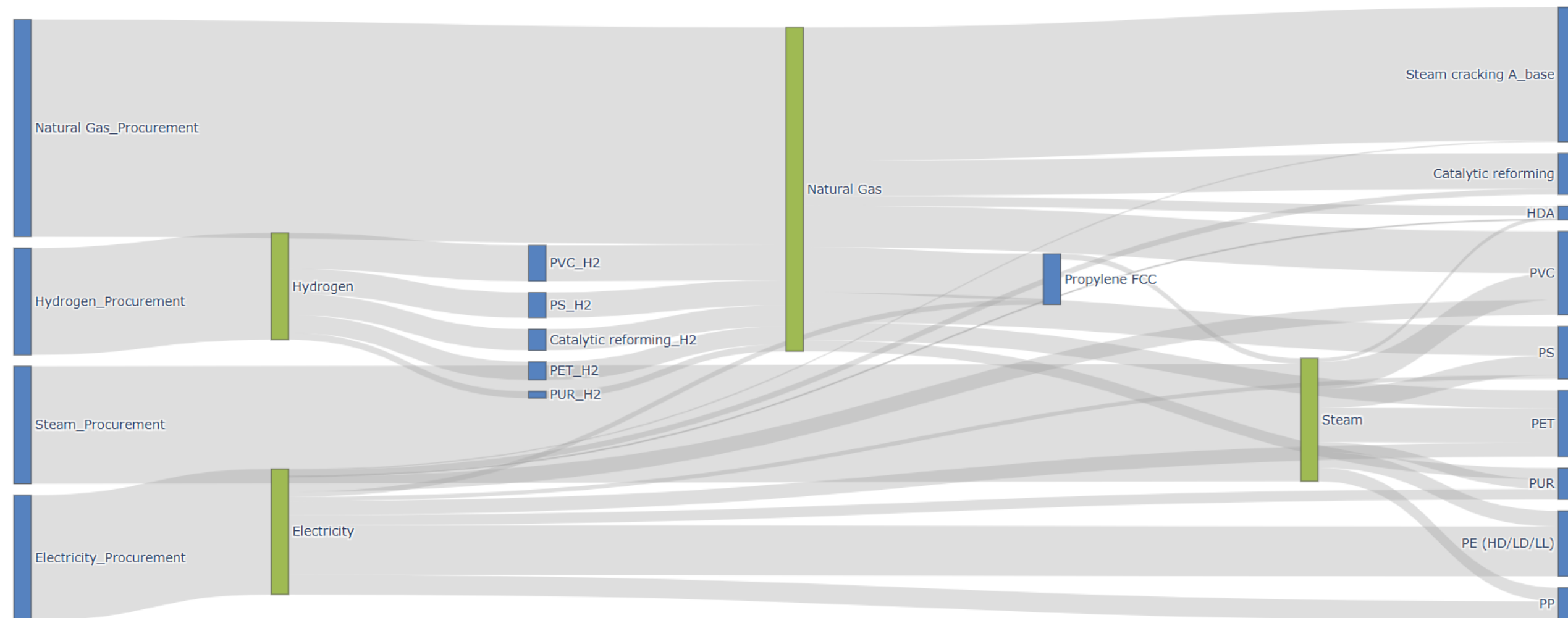
Material flows — 2045 (energy)



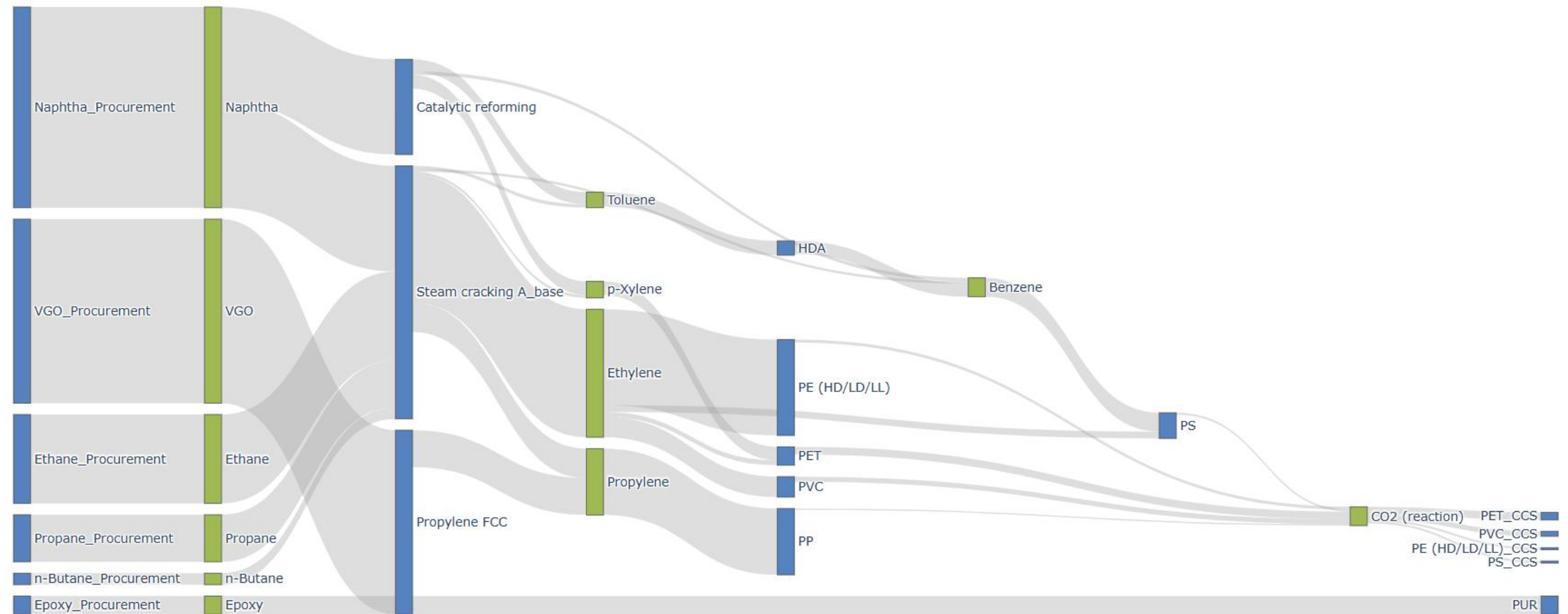
Material flows — 2045 (material)



Material flows — 2050 (energy)



Material flows — 2050 (material)



Annex 2 Model Python code

```

1. # petro_micro.py
2. import re, sys, functools
3. import pandas as pd
4. import pyomo.environ as pyo
5. from pathlib import Path
6. from pyomo.environ import TerminationCondition
7. from pyomo.environ import value
8.
9. # ----- USER SETTINGS -----
10. FILE = "Parameters TFM MII_v2 (1).xlsx" # workbook with
    Parameters & Matrix
11. FREEZE = False # False → simulate 2025-
    2050
12. #
13.
14. # ----- 1. read Parameter sheet + scalar
    helper -----
15. par = (pd.read_excel(FILE, sheet_name="Parameters", header=None)
16.         .fillna(""))
17. par[0] = par[0].astype(str).str.strip()
18. par[1] = (par[1].astype(str).str.strip()
19.           .str.replace("%", "", regex=False)
20.           .replace("", pd.NA).astype(float))
21.
22. def get(label, default=None):
23.     row = par.loc[par[0] == label, 1]
24.     if row.empty:
25.         if default is None:
26.             raise KeyError(f"{label} not found")
27.         return default
28.     return float(str(row.iloc[0]).replace(",", ""))
29.
30. # ----- 2. time axis & staircase
    helper -----
31. yr_pat = re.compile(r"_(20\d{2})$")
32.
33. # ----- helper: split off decarb "family" label -----
    -----

```

```

34.decarb_families = {"H2", "CCS", "Eboiler", "Ecracker"}
35.
36.def split_family(label: str):
37.    """
38.    If the tech name ends with _<family> where family is in
    decarb_families,
39.    return "<prefix>", "<family>". Otherwise (label, None).
40.    """
41.    for fam in decarb_families:
42.        if label.endswith("_" + fam):
43.            return label[: -(len(fam) + 1)], fam    # strip "_<fam>"
44.    return label, None
45.
46.KNOTS = sorted({int(m.group(1)) for lab in par[0]
47.                  if (m := yr_pat.search(str(lab)))})
48.
49.YEAR_FULL = list(range(min(KNOTS), max(KNOTS)+1))
50.YEARS      = [min(KNOTS)] if FREEZE else YEAR_FULL
51.T0         = YEARS[0]
52.
53.def staircase(prefix):
54.    raw = {int(m.group(1)): get(f"{prefix}_{m.group(1)}")
55.            for lab in par[0]
56.            if (m := yr_pat.search(str(lab))) and lab.startswith(prefix)}
57.    cur, full = None, {}
58.    for y in YEARS:
59.        if y in raw:
60.            cur = raw[y]
61.            full[y] = cur
62.    return full
63.
64.grid_EF      = staircase("grid_EF")
65.CO2_price    = staircase("CO2_price")
66.NG_EF       = staircase("Natural Gas_EF")    # tCO2 per GJNG
67.H2_EF       = staircase("Hydrogen_EF")       # tCO2 per GJH2
68.
69.PE_demand_ser = staircase("demand_PE (HD/LD/LL)")
70.PP_demand_ser = staircase("demand_PP")
71.PVC_demand_ser = staircase("demand_PVC")
72.PUR_demand_ser = staircase("demand_PUR")
73.PS_demand_ser = staircase("demand_PS")
74.PET_demand_ser = staircase("demand_PET")
75.

```

```
76._price_cache = {}
77.
78.def price_series(comm):
79.    if comm not in _price_cache:
80.        _price_cache[comm] = staircase(f"{comm}_price")
81.    return _price_cache[comm]
82.
83.# ----- CAPEX staircase (robust matcher) -----
84.# -----
85.@functools.lru_cache(maxsize=None)
86.def capex_series(tech):
87.    """
88.    Forward-fill unit-CAPEX €/t a for *tech*.
89.    1) exact match CAPEX_<yr>_<tech>
90.    2) if not found and tech is incremental (..._H2 / ..._CCS / ..._Eboiler /
..._Ecracker)
91.        fall back to CAPEX_<yr>_<family>
92.    """
93.    raw = {}
94.    prefix, fam = split_family(tech)
95.
96.    for label in par[0]:
97.        if not label.startswith("CAPEX_"):
98.            continue
99.        parts = label.split("_", 2)          # ["CAPEX", "2030",
"<rest>"]
100.        if len(parts) != 3:
101.            continue
102.
103.        year = int(parts[1])
104.        rest = parts[2].strip()
105.
106.        if rest == tech:                    # 1) exact polymer-
specific row
107.            raw[year] = get(label)
108.        elif fam and rest == fam:          # 2) generic family row
109.            # only load generic value if we have no polymer-specific
value yet
110.            # for that year
111.            raw.setdefault(year, get(label))
112.
```

```
113.     cur, full = None, {}
114.     for y in YEARS:
115.         if y in raw:
116.             cur = raw[y]
117.             full[y] = cur if cur is not None else 0.0
118.     return full
119. # -----
-----
120.
121. # ----- Fixed-O&M % (already converted to €/t.a in your sheet) -
-----
122. @functools.lru_cache(maxsize=None)
123. def opex_series(tech):
124.     raw = {}
125.     prefix, fam = split_family(tech)
126.
127.     for label in par[0]:
128.         if not label.startswith("OPEX_"):
129.             continue
130.         parts = label.split("_", 2)
131.         if len(parts) != 3:
132.             continue
133.         year = int(parts[1])
134.         rest = parts[2].strip()
135.
136.         if rest == tech:
137.             raw[year] = get(label)
138.         elif fam and rest == fam:
139.             raw.setdefault(year, get(label))
140.
141.     cur, full = None, {}
142.     for y in YEARS:
143.         if y in raw:
144.             cur = raw[y]
145.             full[y] = cur if cur is not None else 0.0
146.     return full
147. # -----
-----
148.
149. # ---- lifetime resolver -----
-----
150. def tech_life(tech:str, default:int=20) -> int:
151.     """
```

```

152.     Returns the lifetime in years for *tech*.
153.
154.     Resolution order:
155.         1. Life_<exact tech name>
156.         2. Life_<suffix> where suffix is text after the last
           underscore
157.         3. fallback = *default* (20)
158.     """
159.     # (1) exact match
160.     row = par.loc[par[0] == f"Life_{tech}", 1]
161.     if not row.empty and pd.notna(row.iloc[0]):
162.         return int(row.iloc[0])
163.
164.     # (2) generic suffix
165.     suffix = tech.rsplit("_", 1)[-1] # "H2", "Eboiler", "CCS", ...
166.     row = par.loc[par[0] == f"Life_{suffix}", 1]
167.     if not row.empty and pd.notna(row.iloc[0]):
168.         return int(row.iloc[0])
169.
170.     # (3) default
171.     return default
172. # -----
    -----
173.
174. # ----- Ramp staircase (fraction of plastics fleet) -----
    -----
175. @functools.lru_cache(maxsize=None)
176. def ramp_series(label):
177.     """
178.     Return {year: fraction} for rows like Ramp_2030_Eboiler (cell
        value 0.40)
179.     The spreadsheet already stores 15 % as 0.15, so *no extra /100*
        here.
180.     """
181.     raw = {}
182.     for row_lbl in par[0]:
183.         if not row_lbl.lower().startswith("ramp_"):
184.             continue
185.         parts = row_lbl.split("_", 2) # ['Ramp', '2030',
            'Eboiler']
186.         if len(parts) != 3:
187.             continue
188.         _, yr_str, fam = parts

```

```

189.         if fam.strip().lower() != label.lower():
190.             continue
191.         raw[int(yr_str)] = get(row_lbl)           # already a fraction
            (0.15)
192.
193.         # forward-fill
194.         cur, full = 0.0, {}
195.         for y in YEARS:
196.             if y in raw:
197.                 cur = raw[y]
198.                 full[y] = cur
199.         return full
200.     # -----
    -----
201.
202.     # A module-level helper to match the in-model capex_ann logic
203.     def capex_annuity_factor(year, tech):
204.         L = int(get(f"Life_{tech}", 20))
205.         return CRF(L, r) * capex_series(tech)[year]
206.
207.     r = get("real_WACC") / 100
208.
209.     # — helpers that the OBJECTIVE needs —————
210.     def ccs_share(m, t, base_tech, ccs_tech):
211.         """Share of base production routed through the CCS increment
            row."""
212.         def _safe(expr):
213.             x = value(expr, exception=False)
214.             return 0.0 if x is None else x
215.
216.         base_flow = _safe(m.P[t, base_tech])
217.         ccs_flow = _safe(m.P[t, ccs_tech])
218.
219.         return 0.0 if base_flow <= 0 else min(ccs_flow / base_flow, 1.0)
220.
221.     def CRF(life, rate):
222.         """Capital-recovery factor."""
223.         return rate * (1 + rate) ** life / ((1 + rate) ** life - 1)
224.
225.     NZ = 1e-6
226.     r = get("real_WACC")/100
227.

```

```
228. # ----- 3. load & prune Master
    Matrix -----
229. MM_raw = pd.read_excel(FILE, sheet_name="Master Matrix",
    header=None)
230. hdr_idx = MM_raw.index[MM_raw.iloc[:,0]
231.                .str.contains("type", case=False,
    na=False)][0]
232. MM = (pd.read_excel(FILE, sheet_name="Master Matrix", header=hdr_idx)
233.        .loc[:, lambda df: ~df.columns.str.startswith("Unnamed")])
234. MM.columns = MM.columns.str.strip()
235. MM.columns.values[0:2] = ["Type", "Tech"]
236.
237. TECH_KEEP = [
238.     "Steam cracking A_base",
239.     "Steam cracking A_Ecracker",
240.     "Catalytic reforming",
241.     "Catalytic reforming_H2",
242.     "Catalytic reforming_CCS",
243.     "PE (HD/LD/LL)",
244.     "PE (HD/LD/LL)_Eboiler",
245.     "PE (HD/LD/LL)_H2",
246.     "PE (HD/LD/LL)_CCS",
247.     "PP",
248.     "PP_Eboiler",
249.     "PP_H2",
250.     "PP_CCS",
251.     "PVC",
252.     "PVC_Eboiler",
253.     "PVC_H2",
254.     "PVC_CCS",
255.     "PUR",
256.     "PUR_Eboiler",
257.     "PUR_H2",
258.     "PUR_CCS",
259.     "PS",
260.     "PS_Eboiler",
261.     "PS_H2",
262.     "PS_CCS",
263.     "PET",
264.     "PET_Eboiler",
265.     "PET_H2",
266.     "PET_CCS",
267.     "Naphtha_Procurement",
```

```

268.     "Epoxy_Procurement",
269.     "n-Butane_Procurement",
270.     "Propane_Procurement",
271.     "Ethane_Procurement",
272.     "Steam_Procurement",
273.     "Natural Gas_Procurement",
274.     "Electricity_Procurement",
275.     "Hydrogen_Procurement",
276.     "HDA",
277.     "Propylene FCC",
278.     "VGO_Procurement"
279. ]
280. COMM_KEEP = [
281.     "Ethylene", "Electricity", "Steam", "Natural Gas",
282.     "Naphtha", "n-Butane", "Propane", "Ethane",
283.     "PE (HD/LD/LL)", "CO2 (reaction)", "Benzene",
284.     "p-Xylene", "Toluene", "Propylene", "PP", "PVC",
285.     "PUR", "PS", "PET", "Hydrogen", "Epoxy", "VGO"
286. ]
287.
288. MM = (MM[MM["Tech"].isin(TECH_KEEP)]
289.       .loc[:, ["Type", "Tech", *COMM_KEEP]])
290. TECH = MM["Tech"].tolist()
291. COMM = COMM_KEEP.copy()
292. type_of = dict(zip(MM["Tech"], MM["Type"]))
293.
294. # ----- 4. tiny feasibility
295. helper -----
296. def first_violated_constraints(m, *, max_rows=20, tol=1e-6):
297.     from pyomo.environ import value, Constraint
298.     bad = []
299.     for c in m.component_data_objects(Constraint, active=True,
300.         descend_into=True):
301.         if len(bad) >= max_rows:
302.             break
303.         lb = c.lower if c.has_lb() else None
304.         ub = c.upper if c.has_ub() else None
305.         body = value(c.body, exception=False)
306.         if body is None:
307.             continue
308.         if (lb is not None and body < lb - tol) or (ub is not None
309.             and body > ub + tol):
310.             bad.append((c.name, body, lb, ub))

```

```

308.         for n,b,l,u in bad:
309.             print(f"✗ {n:<40} {b:.,.3f} ∉ [{l if l is not None else '-∞'}], "
310.                   f"{u if u is not None else '∞'}]")
311.
312. # — “legacy” CAPEX stream for Cap0
313. def legacy_capex_annuity(m, t):
314.     """
315.     € amortisation in model-year *t* for capacity that existed in
316.     year-0.
317.     We assume 3 equal vintages: built 15, 10 and 5 years before T0.
318.     """
319.     cost = 0.0
320.     for g in m.BASE | m.INCR:
321.         cap0 = m.Cap0[g] if g in m.Cap0.index_set() else 0.0
322.         if cap0 <= 0:
323.             continue
324.         unit_capex = capex_series(g)[T0]           # €/t a for the
325.         Lg          = tech_life(g)                 # design lifetime
326.         share_cap   = cap0 / 3.0                   # each third
327.
328.         for age in (15, 10, 5):                     # years old at T0
329.             start = T0 - age                       # fictitious build
330.             end   = start + Lg                      # when annuity
331.             stops = start + 1                       # still amortising?
332.             if start <= t < end:
333.                 cost += share_cap * unit_capex * CRF(Lg, r)
334.         return cost
335. POLYMERS = ["PE (HD/LD/LL)", "PP", "PVC", "PUR", "PS",
336.             "PET"] # extend this list as you add polymers
337. def polymer_demand(m, poly, t):
338.     if poly == "PE (HD/LD/LL)": return m.demand_PE[t]
339.     elif poly == "PP":          return m.demand_PP[t]
340.     elif poly == "PVC":         return m.demand_PVC[t]
341.     elif poly == "PUR":         return m.demand_PUR[t]
342.     elif poly == "PS":          return m.demand_PS[t]
343.     elif poly == "PET":         return m.demand_PET[t]

```

```

344.         else:                                     return 0.0
345.
346.     # ----- 5. build the Pyomo
347.     model -----
348.     def build_model():
349.         m = pyo.ConcreteModel(name="micro-petro")
350.         # Sets
351.         m.T = pyo.Set(initialize=YEARS, ordered=True)
352.         m.G = pyo.Set(initialize=TECH)
353.         m.I = pyo.Set(initialize=COMM)
354.         m.BASE = pyo.Set(initialize=[g for g in TECH if type_of[g] ==
355.             "Base"])
356.         m.PROC = pyo.Set(initialize=[g for g in TECH if type_of[g] ==
357.             "PROC"])
358.         m.INCR = pyo.Set(initialize=[g for g in TECH if type_of[g] ==
359.             "Increment"])
360.         # Vars
361.         m.P = pyo.Var(m.T, m.G, within=pyo.NonNegativeReals)
362.         m.BuildCap = pyo.Var(m.T, m.BASE | m.INCR,
363.             within=pyo.NonNegativeReals)
364.         m.Cap = pyo.Var(m.T, m.BASE | m.INCR,
365.             within=pyo.NonNegativeReals)
366.         # Params
367.         cap0_dict = {g: get(f"Cap0_{g}", default=0.0) for g in m.BASE |
368.             m.INCR}
369.         m.Cap0 = pyo.Param(m.BASE | m.INCR,
370.             initialize=lambda _, g: cap0_dict[g])
371.         # CO2 PARAMETERS
372.         m.grid_EF = pyo.Param(m.T, initialize=lambda _,t: grid_EF[t])
373.         m.NG_EF = pyo.Param(m.T, initialize=lambda _,t: NG_EF[t])
374.         m.H2_EF = pyo.Param(m.T, initialize=lambda _,t: H2_EF[t])
375.         m.CO2_price = pyo.Param(m.T, initialize=lambda _,t:
376.             CO2_price[t])
377.         # — ramp fractions for each decarb family
378.         -----
379.         ramp_labels = ["Eboiler", "H2", "CCS", "Ecracker"] # plain
380.         list, not dict_values

```

```

376.
377.     # make it a Pyomo Set so you can reference it elsewhere if needed
378.     m.RAMP_LABS = pyo.Set(initialize=ramp_labels)
379.
380.     m.ramp_frac = pyo.Param(
381.         m.T, m.RAMP_LABS,
382.         initialize=lambda _, t, lab: ramp_series(lab)[t]
383.     )
384.
385.     def _alpha(_, g, i):
386.         v = MM.loc[MM["Tech"] == g, i].iloc[0]
387.         return 0.0 if pd.isna(v) else float(v)
388.     m.alpha = pyo.Param(m.G, m.I, initialize=_alpha)
389.
390.     m.price = pyo.Param(
391.         m.T, m.PROC,
392.         initialize=lambda _, t, g: price_series(g.split("_")[0])[t]
393.     )
394.
395.     # €/t·a fixed O&M - forward-filled
396.     m.opex_unit = pyo.Param(
397.         m.T, m.BASE | m.INCR,
398.         initialize=lambda _, t, g: opex_series(g)[t]
399.     )
400.
401.     r = get("real_WACC") / 100
402.     m.DF = pyo.Param(m.T, initialize=lambda _, t: 1/(1+r)**(t-T0))
403.     m.demand_PE = pyo.Param(m.T, initialize=lambda _, t:
404.         PE_demand_ser[t])
405.     m.demand_PP = pyo.Param(m.T, initialize=lambda _, t:
406.         PP_demand_ser[t])
407.     m.demand_PVC = pyo.Param(m.T, initialize=lambda _, t:
408.         PVC_demand_ser[t])
409.     m.demand_PET = pyo.Param(m.T, initialize=lambda _, t:
410.         PET_demand_ser[t])
411.     m.demand_PS = pyo.Param(m.T, initialize=lambda _, t:
412.         PS_demand_ser[t])
413.     m.demand_PUR = pyo.Param(m.T, initialize=lambda _, t:
414.         PUR_demand_ser[t])
415.
416.     # Constraints
417.     FIRST = m.T.first()

```

```

413.     def stock(m, t, g):
414.         base = m.Cap0[g] if t == FIRST else m.Cap[t-1, g]
415.         return m.Cap[t, g] == base + m.BuildCap[t, g]
416.     m.Stock = pyo.Constraint(m.T, m.BASE | m.INCR, rule=stock)
417.
418.     def cap_lim(m, t, g):
419.         return m.P[t, g] <= m.Cap[t, g] if (g in m.BASE | m.INCR) \
420.             else pyo.Constraint.Skip
421.     m.CapLim = pyo.Constraint(m.T, m.G, rule=cap_lim)
422.
423.     def follow_base(m, t, g_incr):
424.         # extract the corresponding base technology name
425.         g_base = g_incr.split("_")[0].strip() # "PE
(HD/LD/LL)"
426.         if g_base not in m.G: # safety
427.             return pyo.Constraint.Skip
428.         # run increment only if base is running (allow ≤, not =, so
optimiser can stay below the ramp)
429.         return m.P[t, g_incr] <= m.P[t, g_base]
430.
431.     m.FollowBase = pyo.Constraint(m.T, m.INCR, rule=follow_base)
432.
433.     # ----- polymer-specific CCS / H2 / E-boiler ramp
-----
434.     #
435.     # Ramp target applies separately to each "polymer family"
436.     # PE, PP, PVC, PUR, PS, PET, ...
437.     # Shared ramp percentages (5 %, 10 %, ...) still come from the
Ramp_* rows.
438.
439.     def prefix_of(g):
440.         """return polymer name without trailing '_CCS' / '_H2' / ..."""
441.         for fam in m.RAMP_LABS: # CCS, H2, ...
442.             suf = "_" + fam
443.             if g.endswith(suf):
444.                 return g[:-len(suf)]
445.         return g # base rows
446.
447.     # gather all prefixes that **have** a ramp-eligible row
448.     poly_prefixes = sorted({prefix_of(g) for g in m.G
449.                             if any(g.endswith(lab) for lab in
m.RAMP_LABS)})
450.

```

```

451.     m.POLY = pyo.Set(initialize=poly_prefixes)           # e.g. "PE
      (HD/LD/LL)", "PP", ...
452.
453.     def ramp_limit_poly(m, t, poly, lab):
454.         """
455.          $\sum \text{Cap}(\text{incr rows of } \langle \text{poly} \rangle \ \& \ \langle \text{lab} \rangle) \leq \text{ramp\%} \cdot \text{Cap}(\langle \text{poly} \rangle \text{ base}$ 
      row)
456.         """
457.         base_tech = poly
458.         if base_tech not in m.G:                           # safety for exotic
      names
459.             return pyo.Constraint.Skip
460.
461.         incr_cap = sum(m.Cap[t, g]
462.                        for g in m.INCR
463.                        if g.startswith(poly + "_") and g.endswith(lab))
464.
465.         return incr_cap <= m.ramp_frac[t, lab] * m.Cap[t, base_tech]
466.
467.         # one 3-index constraint: (year, polymer family, lab)
468.         m.RampPoly = pyo.Constraint(m.T, m.POLY, m.RAMP_LABS,
      rule=ramp_limit_poly)
469.
470.     def bal_poly(m, t, poly):
471.         """
472.         Mass balance for each finished polymer.
473.         For PE and PP we enforce >= their respective external demand
      series.
474.         """
475.         lhs = sum(m.alpha[g, poly] * m.P[t, g]              # net
      production
476.                  for g in m.G)
477.         rhs = polymer_demand(m, poly, t)                    # exogenous
      demand
478.         return lhs >= rhs
479.
480.     m.BalPoly = pyo.Constraint(m.T, POLYMERS, rule=bal_poly)
481.
482.     def bal_other(m, t, i):
483.         if i in POLYMERS:                                   # skip PE, PP, ... (any future
      polymers)
484.             return pyo.Constraint.Skip

```

```

485.         return sum(m.alpha[g, i] * m.P[t, g] for g in m.G) >= 0
486.     m.Bal = pyo.Constraint(m.T, m.I, rule=bal_other)
487.
488.     # Objective
489.     def capex_ann(y, g):
490.         L = tech_life(g)
491.         CRF = r*(1+r)**L/((1+r)**L - 1)
492.         return capex_series(g)[y] * CRF
493.
494.     def annual_cost(m, t):
495.         # 1) feed / energy purchases
496.         buy_cost = sum(m.price[t, g] * m.P[t, g] for g in m.PROC)
497.
498.         # 2) capex annuities (Base + Increment)
499.         cap_cost = sum(
500.             capex_ann(y, g) * m.BuildCap[y, g]
501.             for g in (m.BASE | m.INCR)
502.             for y in m.T
503.             if y <= t < y + tech_life(g)
504.         )
505.
506.         # 3) annuities of the LEGACY fleet
507.         cap_cost_legacy = legacy_capex_annuity(m, t)
508.
509.         # 3) fixed-O&M (€/t a * installed cap)
510.         fom_cost = sum(
511.             m.opex_unit[t, g] * m.Cap[t, g]
512.             for g in (m.BASE | m.INCR)
513.         )
514.
515.         # 4) direct-process CO2
516.         direct_co2_cost = (
517.             sum(m.alpha[g, "CO2 (reaction)"] * m.P[t, g] for g in
518.                 m.G)
519.             * m.CO2_price[t]
520.         )
521.
522.         # 5) electricity CO2
523.         elec_co2_cost = (
524.             m.P[t, "Electricity_Procurement"] * m.grid_EF[t] *
525.             m.CO2_price[t]
526.             if "Electricity_Procurement" in m.PROC else 0.0
527.         )

```

```

526.
527.     # 6) fuel & steam CO2 (NG part is partially captured by CCS)
528.     # -----
529.     def captured(frac):
530.         """apply NG-capture share from CCS retrofits"""
531.         return frac * (
532.             1.0 - ccs_share(m, t,
533.                             "PE (HD/LD/LL)",          # base row
534.                             "PE (HD/LD/LL)_CCS")        # CCS row
535.             )
536.
537.         fuel_tCO2 = 0.0
538.         if "Natural Gas_Procurement" in m.PROC:
539.             fuel_tCO2 += captured(m.P[t, "Natural Gas_Procurement"] *
540.                                  m.NG_EF[t])
541.         if "Hydrogen_Procurement" in m.PROC:
542.             fuel_tCO2 += m.P[t, "Hydrogen_Procurement"] * m.H2_EF[t]
543.
544.         steam_tCO2 = 0.0
545.         if "Steam_Procurement" in m.PROC:          # NG-boiler
546.             steam
547.             steam_tCO2 = captured(m.P[t, "Steam_Procurement"] *
548.                                   m.NG_EF[t])
549.
550.         fuel_co2_cost = fuel_tCO2 * m.CO2_price[t]
551.         steam_co2_cost = steam_tCO2 * m.CO2_price[t]
552.
553.         # total
554.         return (
555.             buy_cost + cap_cost + fom_cost + direct_co2_cost +
556.             elec_co2_cost
557.             + fuel_co2_cost + steam_co2_cost + cap_cost_legacy
558.             )
559.
560.     m.Obj = pyo.Objective(expr=sum(m.DF[t]*annual_cost(m,t) for t in
561.                                     m.T),
562.                           sense=pyo.minimize)
563.
564.     # — make the helper visible outside build_model —————
565.     m.annual_cost = annual_cost          # <— add this line
566.
567.     return m

```

```

564. # ----- 6. solve &
      diagnostics -----
565. if __name__ == "__main__":
566.     m = build_model()
567.
568.     # quick peek
569.     print("Initial capacities (Cap0):")
570.     for g in m.G:
571.         if g in m.Cap0.index_set():
572.             print(f" {g:<30} {pyo.value(m.Cap0[g]):,.0f}")
573.         else:
574.             print(f" {g:<30} (no Cap0 entry)")
575.
576.     from pyomo.environ import Suffix
577.     m.rc = Suffix(direction=Suffix.IMPORT) # reduced cost (=
      shadow price)
578.
579.     res = pyo.SolverFactory("gurobi").solve(m, tee=True)
580.     if res.solver.termination_condition !=
      TerminationCondition.optimal:
581.         print("⚠ Model not optimal")
582.         first_violated_constraints(m)
583.         sys.exit(1)
584.
585.     # — helpers
      -----
586.     def safe(v):
587.         """Return numeric value of a Pyomo var/expr; 0.0 if None."""
588.         x = value(v, exception=False)
589.         return 0.0 if x is None else x
590.
591.     def var_to_df(comp, idx_names):
592.         rows = []
593.         for k, v in comp.items():
594.             rows.append((*(k if isinstance(k, tuple) else (k,)),
      safe(v)))
595.         return pd.DataFrame(rows, columns=[*idx_names, "value"])
596.
597.     rows = []
598.     for t in m.T:
599.         for poly in POLYMERS:
600.             prod = sum(m.alpha[g, poly] * safe(m.P[t, g]) for g in
      m.G)

```

```

601.         rows.append((t, poly, prod, polymer_demand(m, poly, t)))
602.
603.     balance_all = pd.DataFrame(
604.         rows, columns=["year", "polymer", "produced", "demand"]
605.     ).sort_values(["year", "polymer"])
606.
607.     # 2. other balances
608.     COM_SHOW = [ "Ethylene", "Electricity", "Steam", "Natural Gas",
609.         "Naphtha", "n-Butane", "Propane", "Ethane", "Benzene",
610.         "p-Xylene", "Toluene", "Propylene", "Hydrogen", "Epoxy" ]
611.     cb = pd.DataFrame([(t,i,sum(m.alpha[g, i] * safe(m.P[t, g])
612.         for g in m.G))
613.         for t in m.T for i in COM_SHOW],
614.         columns=["year","comm","net"])
615.     print("\n► OTHER COMMODITY BALANCES (≥0)")
616.     print(cb.pivot(index="year",columns="comm",values="net"))
617.
618.     # 3. procurement
619.     buy_df = (var_to_df(m.P,["year","tech"])
620.         .query("tech.str.endswith('_Procurement')",engine="pyth
621.         on")
622.         .pivot(index="year",columns="tech",values="value").fill
623.         na(0))
624.     print("\n► PROCUREMENT FLOWS"); print(buy_df)
625.
626.     # 4. utilisation
627.     util_df = pd.DataFrame(
628.         [
629.             (t, g,
630.             safe(m.P[t, g]),
631.             safe(m.Cap[t, g]))
632.             for t in m.T
633.             for g in [ "Steam cracking A_base",
634.             "Steam cracking A_Ecracker",
635.             "Catalytic reforming",
636.             "Catalytic reforming_H2",
637.             "Catalytic reforming_CCS",
638.             "PE (HD/LD/LL)",
639.             "PE (HD/LD/LL)_Eboiler",
640.             "PE (HD/LD/LL)_H2",
641.             "PE (HD/LD/LL)_CCS",
642.             "PP",
643.             "PP_Eboiler",

```

```

642.     "PP_H2",
643.     "PP_CCS",
644.     "PVC",
645.     "PVC_Eboiler",
646.     "PVC_H2",
647.     "PVC_CCS",
648.     "PUR",
649.     "PUR_Eboiler",
650.     "PUR_H2",
651.     "PUR_CCS",
652.     "PS",
653.     "PS_Eboiler",
654.     "PS_H2",
655.     "PS_CCS",
656.     "PET",
657.     "PET_Eboiler",
658.     "PET_H2",
659.     "PET_CCS",
660.     "HDA",
661.     "Propylene FCC"]
662.     ],
663.     columns=["year", "tech", "P", "Cap"]
664. )
665.
666. # — RAMP-check —————
667. ramp_chk = []
668. for t in m.T:
669.     base_cap = sum( safe(m.Cap[t,g]) for g in m.BASE )
670.     for lab in m.RAMP_LABS:
671.         incr_cap = sum( safe(m.Cap[t,g]) for g in m.INCR if
672.             g.endswith(lab) )
673.         ramp_chk.append((
674.             t, lab,
675.             incr_cap,
676.             m.ramp_frac[t, lab],
677.             incr_cap / base_cap if base_cap > 0 else 0
678.         ))
679. ramp_df = pd.DataFrame(
680.     ramp_chk,
681.     columns=["year", "family", "incr_cap", "ramp_limit", "share"]
682. )
683. print("\n► RAMP VERIFICATION")
684. print(ramp_df)

```

```

684.
685.     # 5. capacity builds & CAPEX
686.     cap_rows=[]
687.     for t in m.T:
688.         for g in m.BASE | m.INCR:
689.             add = safe(m.BuildCap[t, g])
690.             if add<=NZ: continue
691.             life=int(get(f"Life_{g}",20))
692.             unit=capex_series(g)[t]
693.             cap_rows.append((t,g,add,unit,add*unit,add*unit*CRF(life,
r)))
694.
695.     # ----- LEGACY-fleet "amortization" -----
696.     if t == T0:
697.         for g in m.BASE | m.INCR:
698.             cap0 = m.Cap0[g]
699.             if cap0 <= NZ:
700.                 continue
701.             life = tech_life(g)
702.             unit = capex_series(g)[T0]
703.             for rem, share in [(5,1/3), (10,1/3), (15,1/3)]:
704.                 eff_cap = cap0 * share * rem / life
705.                 ann      = eff_cap * unit * CRF(life, r)
706.                 cap_rows.append((T0,
707.                                 f"{g} (legacy, {rem} y left)",
708.                                 eff_cap, unit, eff_cap*unit, ann))
709.
710.     capex_df=pd.DataFrame(cap_rows,
711.                           columns=["year","tech","capacity_added","unit_capex",
712.                                   "total_capex","annuity_capex"]).sort_values(["year",
"tech"])
713.     print("\n► CAPACITY BUILDS")
714.     print("(none)" if capex_df.empty else capex_df)
715.
716.     # 6. Yearly cost breakdown
717.     energy_procs = {
718.         "Steam_Procurement",
719.         "Hydrogen_Procurement",
720.         "Natural Gas_Procurement",
721.         "Electricity_Procurement",
722.     }
723.

```

```

724. cost_rows = []
725. for t in m.T:
726.
727.     # — 1) split feed purchases into RAW vs ENERGY
       _____
728.     feed_raw_cost = 0.0 # materials (naphtha, butane, ...)
729.     feed_energy_cost = 0.0 # Steam, NG, H2, Electricity
730.     for proc in m.PROC:
731.         cost = m.price[t, proc] * safe(m.P[t, proc])
732.         if proc in energy_procs:
733.             feed_energy_cost += cost
734.         else:
735.             feed_raw_cost += cost
736.
737.     # — 2) capex annuities still outstanding
       _____
738.     cap_stream = 0.0
739.     for g in (m.BASE | m.INCR):
740.         Lg = tech_life(g)
741.         for y in m.T:
742.             if y <= t < y + Lg:
743.                 cap_stream += (
744.                     capex_annuity_factor(y, g) * safe(m.BuildCap[y,
745. g])
746.                 )
747.     # ----- legacy annuity -----
748.     for g in (m.BASE | m.INCR):
749.         cap0 = m.Cap0[g] if g in m.Cap0.index_set() else 0.0
750.         if cap0 <= 0:
751.             continue
752.         life = tech_life(g)
753.         CRF0 = CRF(life, r)
754.         ann0 = cap0 * capex_series(g)[T0] * CRF0
755.         # remaining life fractions: 1/3 for 5 y left, etc.
756.         rem_ann = (ann0/3) * (life-5)/life + (ann0/3) * (life-
10)/life + (ann0/3) * (life-0)/life
757.         cap_stream += rem_ann
758.
759.     # — 3) direct-process CO2 (from “CO2 (reaction)” column)
       _____
760.     if "CO2 (reaction)" in m.I:
761.         direct_tCO2 = sum(

```

```

762.         m.alpha[g, "CO2 (reaction)"] * safe(m.P[t, g])
763.         for g in m.G
764.     )
765.     direct_CO2_cost = direct_tC02 * m.CO2_price[t]
766. else:
767.     direct_CO2_cost = 0.0
768.
769.     # — 4) electricity CO2 cost
    -----
770.     elec_CO2_cost = (
771.         safe(m.P[t, "Electricity_Procurement"])
772.         * m.grid_EF[t] * m.CO2_price[t]
773.         if "Electricity_Procurement" in m.PROC
774.         else 0.0
775.     )
776.
777.     # — 5) fuel CO2 cost (NG + H2)
    -----
778.     fuel_tC02 = 0.0
779.     for proc in ("Natural Gas_Procurement", "Hydrogen_Procurement"):
780.         if proc in m.PROC:
781.             ef = m.NG_EF[t] if proc.startswith("Natural Gas") else
m.H2_EF[t]
782.             raw = safe(m.P[t, proc]) * ef                # ► emissions
*before* CCS
783.             # ----- CCS capture share -----
-----
784.             if proc.startswith("Natural Gas"):           # only NG is
captured
785.                 share = ccs_share(m, t,
786.                                     "PE (HD/LD/LL)",      # base row
787.                                     "PE (HD/LD/LL)_CCS")    # CCS row
788.                 raw *= (1.0 - share)                      # subtract captured
part
789.                 fuel_tC02 += raw
790.             fuel_CO2_cost = fuel_tC02 * m.CO2_price[t]
791.
792.     # — 6) steam CO2 cost (assuming NG boiler)
    -----
793.     steam_raw_tC02 = (
794.         safe(m.P[t, "Steam_Procurement"]) * m.NG_EF[t]
795.         if "Steam_Procurement" in m.PROC else 0.0
796.     )

```

```

797.     steam_CO2_cost = (
798.         steam_raw_tCO2 * (1.0 - ccs_share(m, t,
799.             "PE (HD/LD/LL)",
800.             "PE (HD/LD/LL)_CCS"))
801.         * m.CO2_price[t]
802.     )
803.
804.     # — 7) FOM costs —————
805.     fom_cost = sum(
806.         m.opex_unit[t, g] * safe(m.Cap[t, g])
807.         for g in (m.BASE | m.INCR)
808.     )
809.
810.     # — 7) total cost for year t
811.     total = (
812.         feed_raw_cost
813.         + feed_energy_cost
814.         + cap_stream
815.         + direct_CO2_cost
816.         + elec_CO2_cost
817.         + fuel_CO2_cost
818.         + steam_CO2_cost
819.         + fom_cost
820.     )
821.
822.     cost_rows.append((
823.         t,
824.         feed_raw_cost,
825.         feed_energy_cost,
826.         cap_stream,
827.         fom_cost,
828.         direct_CO2_cost,
829.         elec_CO2_cost,
830.         fuel_CO2_cost,
831.         steam_CO2_cost,
832.         total
833.     ))
834.
835.     # Build DataFrame *after* the loop
836.     cost_df = pd.DataFrame(
837.         cost_rows,
838.         columns=[

```

```
839.         "year",
840.         "feed_raw_cost",
841.         "feed_energy_cost",
842.         "capex_annuity",
843.         "fom_cost",
844.         "direct_CO2_cost",
845.         "elec_CO2_cost",
846.         "fuel_CO2_cost",
847.         "steam_CO2_cost",
848.         "total_cost",
849.     ]
850. )
851.
852. # — 6-bis. Fixed-OPEX diagnostics
853. opex_rows = []
854. for t in m.T:
855.     for g in (m.BASE | m.INCR):
856.         cap = safe(m.Cap[t, g])
857.         if cap <= NZ:
858.             continue
859.         unit = m.opex_unit[t, g] # €/t a
860.         opex_rows.append((t, g, cap, unit, cap * unit))
861.
862. opex_df = (
863.     pd.DataFrame(
864.         opex_rows,
865.         columns=[
866.             "year",
867.             "tech",
868.             "installed_cap",
869.             "unit_opex_eur_per_tpa",
870.             "opex_cost_eur",
871.         ],
872.     )
873.     .sort_values(["year", "tech"])
874. )
875. print("\n► OPEX COSTS"); print(opex_df.head())
876.
877. # — one-time definition, above 7-bis
878. from pathlib import Path
879. out = Path("micro_diagnostics.xlsx")
880. try:
```

```

881.     import xlswriter; engine = "xlswriter"
882. except ImportError:
883.     import openpyxl;     engine = "openpyxl"
884. # -----
885.
886. # -----
887. # 7-bis  ADD-1-TONNE  (Base **plus** Increment)  - every 5 years -
888. # -----
889.
889. from pyomo.environ import value
890.
891. def safe(v):
892.     x = value(v, exception=False)
893.     return 0.0 if x is None else x
894.
895. # ---- (1) full-year cost exactly as the objective sees it -----
896.
896. def year_cost(t):
897.     tot = 0.0
898.
899.     # 1) purchases
900.     for g in m.PROC:
901.         tot += m.price[t, g] * safe(m.P[t, g])
902.
903.     # 2) CAPEX annuity + FOM + legacy
904.     for g in (m.BASE | m.INCR):
905.         L = tech_life(g)
906.         CRF = r * (1 + r) ** L / ((1 + r) ** L - 1)
907.         for y in m.T:
908.             if y <= t < y + L:
909.                 tot += CRF * capex_series(g)[y] * safe(m.BuildCap[y,
910. g])
911.                 tot += m.opex_unit[t, g] * safe(m.Cap[t, g])
912.
912.     # 3) direct-process CO2
913.     co2_dir = sum(
914.         m.alpha[g, "CO2 (reaction)"] * safe(m.P[t, g]) for g in m.G
915.     )
916.     tot += co2_dir * m.CO2_price[t]
917.
918.     # 4) grid-electricity CO2

```

```

919.         if "Electricity_Procurement" in m.PROC:
920.             elec = safe(m.P[t, "Electricity_Procurement"])
921.             tot += elec * m.grid_EF[t] * m.CO2_price[t]
922.
923.         # 5) fuel + steam CO2 **<-- ADD THIS SECTION**
924.         fuel_tCO2 = 0.0
925.         if "Natural Gas_Procurement" in m.PROC:
926.             fuel_tCO2 += safe(m.P[t, "Natural Gas_Procurement"]) *
m.NG_EF[t]
927.         if "Hydrogen_Procurement" in m.PROC:
928.             fuel_tCO2 += safe(m.P[t, "Hydrogen_Procurement"]) *
m.H2_EF[t]
929.
930.         steam_tCO2 = 0.0
931.         if "Steam_Procurement" in m.PROC:
932.             steam_tCO2 += safe(m.P[t, "Steam_Procurement"]) * m.NG_EF[t]
933.
934.         tot += (fuel_tCO2 + steam_tCO2) * m.CO2_price[t]
935.
936.         return float(tot)
937.
938.     # ---- (2) utility shifter -----
-----
939.     DRIVERS = ["Natural Gas", "Hydrogen", "Steam", "Electricity"]
940.     UT_PROC = {d: f"{d}_Procurement" for d in DRIVERS}
941.
942.     def shift_utils(t, row, tonnes):
943.         Δ = {}
944.         for drv, proc in UT_PROC.items():
945.             if proc not in m.PROC:                # not modelled → skip
946.                 continue
947.             coeff = m.alpha[row, drv] if (row, drv) in
m.alpha.index_set() else 0
948.             dP = -coeff * tonnes
949.             if abs(dP) > 1e-9:
950.                 cur = safe(m.P[t, proc])
951.                 m.P[t, proc].set_value(cur + dP)
952.                 Δ[proc] = dP
953.         return Δ
954.
955.     # ---- (3) provision just-enough name-plate -----
-----
956.     def add_cap(t, row, tonnes):

```

```

957.     cap = safe(m.Cap[t, row]);    flow = safe(m.P[t, row])
958.     util = flow / cap if cap > 0 else 0.85
959.     util = max(util, 0.10)                # floor 10 %
960.     spare = cap - flow
961.     need = max(0.0, tonnes - spare) / util
962.     if need > 0:
963.         m.BuildCap[t,row].set_value(safe(m.BuildCap[t,row]) + need)
964.         m.Cap[t,row].set_value(cap + need)
965.     return need
966.
967. # ---- (4) incremental cost routine (Base **plus** Increment) ----
    -----
968. def add_cost(t, g_incr, tonnes=1.0):
969.     vars_ = [m.P[t,g_incr], m.BuildCap[t,g_incr], m.Cap[t,g_incr]]
970.     snap = [v.value for v in vars_]
971.
972.     add_cap(t, g_incr, tonnes)
973.     util = shift_utils(t, g_incr, +tonnes)
974.     m.P[t, g_incr].set_value(snap[0] + tonnes)
975.
976.     after = year_cost(t)
977.
978.     # rollback
979.     for v,val in zip(vars_, snap):
980.         v.set_value(val)
981.     for p,dP in util.items():
982.         m.P[t,p].set_value(safe(m.P[t,p]) - dP)
983.
984.     before = year_cost(t)
985.     return (after - before) / tonnes
986.
987. # ---- (5) build table every 5th year -----
    -----
988. rows = []
989. for t in m.T:
990.     if (t - T0) % 5:                # keep only 25/30/35/...
991.         continue
992.
993.     # polymer-specific decarb families
994.     for poly in POLYMERS:            # e.g. PE, PP, PVC ...
995.         for fam in ["CCS","Eboiler","H2"]:
996.             g_incr = f"{poly}_{fam}"
997.             if g_incr not in m.G:

```

```

998.         continue
999.         rows.append((t, poly, fam,
1000.                    add_cost(t, g_incr, 1.0)))
1001.
1002.     # the generic E-cracker (not tied to one polymer)
1003.     if "Steam cracking A_Ecracker" in m.G:
1004.         rows.append((t, "-", "Ecracker",
1005.                    add_cost(t, "Steam cracking A_Ecracker", 1.0)))
1006.
1007. incr_df = (pd.DataFrame(rows,
1008.                        columns=["year", "polymer", "family", "incremental_cost_€/t"
1009.                                ]))
1010.
1011.         .sort_values(["year", "polymer", "family"]))
1012.
1011. # — NEW: decarbonisation-family capacity
1012. overview —————
1012. decarb_rows = []
1013. families = ["H2", "CCS", "Eboiler", "Ecracker"] # keep in sync
1014. with model
1014. for t in m.T:
1015.     for fam in families:
1016.         cap_sum = sum(
1017.             safe(m.Cap[t, g])
1018.             for g in m.INCR
1019.             if g.endswith(fam) # match family
1020.         )
1021.         decarb_rows.append((t, fam, cap_sum))
1022.
1023. decarb_cap_df = pd.DataFrame(
1024.     decarb_rows, columns=["year", "family", "installed_cap_tpa"]
1025. ).sort_values(["year", "family"])
1026. print("\n► INSTALLED CAPACITY BY DECARB
1027.     FAMILY"); print(decarb_cap_df.head())
1028.
1028. # -----
1029. # keep only milestone years (every 5th year starting with T0 = 2025)
1030. # -----
1031. MILESTONE_YEARS = [y for y in m.T if (y - T0) % 5 == 0]
1032.
1033. def only_milestones(df, year_col="year"):
1034.     """Return *df* filtered to rows/index belonging to
1035.     MILESTONE_YEARS."""

```

```

1035.     if year_col in df.columns:
1036.         return df[df[year_col].isin(MILESTONE_YEARS)].copy()
1037.     elif df.index.name == year_col:                                     # e.g. pivot
1038.         tables
1039.         return df.loc[MILESTONE_YEARS].copy()
1040.     else:
1041.         # DataFrames that have year in the index but no label
1042.         try:
1043.             return df.loc[MILESTONE_YEARS].copy()
1044.         except KeyError:
1045.             return df                                                    # leave
1046.         untouched
1047. # 7. Excel export
1048. with pd.ExcelWriter(out, engine=engine) as w:
1049.     only_milestones(balance_all) \
1050.         .to_excel(w, sheet_name="PE_balance", index=False)
1051.     only_milestones(cb) \
1052.         .to_excel(w, sheet_name="comm_balances", index=False)
1053.     only_milestones(buy_df, year_col="year") \
1054.         .to_excel(w, sheet_name="purchases", index=True)
1055.     only_milestones(util_df) \
1056.         .to_excel(w, sheet_name="utilisation", index=False)
1057.     only_milestones(capex_df) \
1058.         .to_excel(w, sheet_name="capacity_build", index=False)
1059.     only_milestones(decarb_cap_df) \
1060.         .to_excel(w, sheet_name="decarb_family_cap", index=False)
1061.     only_milestones(cost_df) \
1062.         .to_excel(w, sheet_name="annual_costs", index=False)
1063.     only_milestones(opex_df) \
1064.         .to_excel(w, sheet_name="opex_costs", index=False)
1065.     only_milestones(incr_df) \
1066.         .to_excel(w,
1067.             sheet_name="incremental_costs", index=False)
1068.

```

```

1075.     if engine == "xlsxwriter":
1076.         util_ws = w.sheets["utilisation"]
1077.         util_ws.conditional_format(
1078.             f"D2:D{len(util_df)+1}",
1079.             {"type": "3_color_scale"}
1080.         )
1081.
1082. print("🔗 BASE rows:", [g for g in m.BASE if g.endswith("CCS")])
1083. print("🔗 INCR rows:", [g for g in m.INCR if g.endswith("CCS")])
1084.
1085. print(f"\n📁 Diagnostics written to {out.resolve()}")
1086. #

```

```

1087. # 8. S A N K E Y   P L O T T E R   (v2.1)
1088. #     three flavours per "mode":
1089. #         mode="material"    - only non-energy material flows
1090. #         mode="energy"     - only Steam / Elec / NG / H2 (+ their
1091. #         mode="combined"   - everything together
1092. #

```

```

1093. def sankey_year(
1094.     t: int = 2030,
1095.     mode: str = "material",          # "material" | "energy" |
    "combined"
1096.     top_n: int | None = 40,          # keep biggest |flow|; None
    = all
1097.     min_flow: float = 0.5,           # hide flows < min_flow kt
1098.     outfile: str | None = None,
1099.     kt: bool = True
1100. ):
1101.     """
1102.     Interactive Sankey for model-year *t* with a fixed 7-column
    layout:
1103.
1104.     0  Procurement rows    (..._Procurement)
1105.     1  Primary feedstocks (Naphtha, VGO, Ethane, n-Butane,
    Propane, Epoxy)
1106.     2  Process units      (Steam-cracker, FCC, Cat-reforming, HDA
    ...)

```

```

1107.      3 Intermediates & energy carriers (ethylene, steam,
      electricity ...)
1108.      4 Polymers          (PE, PP, PVC, PUR, PS, PET)
1109.      5 CO2 (reaction)
1110.      6 *_CCS rows        (one per polymer)
1111.
1112.      *mode* chooses which links are kept **per flow** (not per node):
1113.      - "material": drop any link that touches an energy carrier
1114.      - "energy"   : keep only links that touch an energy carrier
1115.      - "combined": show everything
1116.      ""
1117.
1118.      # — helper sets
      _____
1119.      clean = lambda s: str(s).strip()
1120.
1121.      feedstocks      = {clean(x) for x in
1122.          ["Naphtha", "VGO", "Ethane", "n-Butane", "Propane", "Epoxy"]}
1123.
1124.      energy_carriers  = {clean(x) for x in
1125.          ["Electricity", "Steam", "Natural Gas", "Hydrogen"]}
1126.
1127.      polymers         = {clean(x) for x in POLYMERS}
1128.
1129.      processes_extra   = {"HDA"}           # force to column 2
1130.      intermediates_extra = {"Benzene"}     # force to column 3
1131.
1132.      # — column classifier
      _____
1133.      def column_of(node: str) -> int:
1134.          n = clean(node)
1135.
1136.          if n.endswith("_Procurement"):      return 0
1137.          if n in feedstocks:                  return 1
1138.          if n in polymers:                    return 4
1139.          if n == "CO2 (reaction)":            return 5
1140.          if n.endswith("_CCS"):               return 6
1141.          if n in processes_extra or (n in TECH and
1142.              not n.endswith("_Procurement"))
1143.              and
1144.              not
1145.              n.endswith("_CCS")):            return 2
1146.          # energy carriers & all other intermediates

```

```

1145.         return 3
1146.
1147.     # — quick helpers -----
1148.     def is_energy(node: str) -> bool:
1149.         n = clean(node)
1150.         return (n in energy_carriers or
1151.                 (n.endswith("_Procurement")
1152.                  and n.split("_")[0] in energy_carriers))
1153.
1154.     def flow_kept(src: str, dst: str) -> bool:
1155.         """Decide whether the *link* (src→dst) survives the mode
1156.         filter."""
1157.         if mode == "material":
1158.             return not (is_energy(src) or is_energy(dst))
1159.         if mode == "energy":
1160.             return (is_energy(src) or is_energy(dst))
1161.         return True # combined
1162.
1163.     # — 1. gather gross flows F_{tech→comm} =
1164.      $\alpha \cdot P$ 
1165.     flows: list[tuple[str, str, float]] = []
1166.
1167.     for g in m.G:
1168.         Pg = safe(m.P[t, g])
1169.         if Pg <= 0:
1170.             continue
1171.         for i in COMM:
1172.             coeff = m.alpha[g, i]
1173.             if abs(coeff) <= 1e-12:
1174.                 continue
1175.             q = coeff * Pg # sign preserved
1176.             (t/yr)
1177.
1178.             if abs(q) < min_flow * 1_000: # kt threshold
1179.                 continue
1180.
1181.             src, dst, val = (
1182.                 (clean(g), clean(i), +q) if q > 0 else
1183.                 (clean(i), clean(g), -q) )
1184.
1185.             if src == dst:
1186.                 continue # drop self-loops

```

```

1184.
1185.         if not flow_kept(src, dst):
1186.             continue
1187.
1188.         flows.append((src, dst, val))
1189.
1190.     if not flows:
1191.         print(f"⚠ No flows survive filters for year {t} "
1192.               f"in mode \"{mode}\".")
1193.         return
1194.
1195.     # keep only the largest |flow|s
1196.     if top_n is not None:
1197.         flows = sorted(flows, key=lambda x: -x[2])[:top_n]
1198.
1199.     # — 2. build the ordered node list -----
1200.     col_nodes: dict[int, list[str]] = {c: [] for c in range(7)}
1201.     seen: set[str] = set()
1202.
1203.     for s, d, _ in flows:
1204.         for n in (s, d):
1205.             if n not in seen:
1206.                 col_nodes[column_of(n)].append(n)
1207.                 seen.add(n)
1208.
1209.     # stable alphabetical ordering within each column
1210.     nodes: list[str] = []
1211.     for col in range(7):
1212.         nodes.extend(sorted(col_nodes[col], key=str.casefold))
1213.
1214.     idx = {n: k for k, n in enumerate(nodes)}
1215.
1216.     # — 3. Plotly figure -----
1217.     import plotly.graph_objects as go
1218.
1219.     scale = 1_000 if kt else 1
1220.     unit = "kt" if kt else "t"
1221.
1222.     fig = go.Figure(
1223.         go.Sankey(
1224.             arrangement="snap",

```

```

1225.         node=dict(
1226.             pad=10, thickness=15,
1227.             label=nodes,
1228.             color=[
1229.                 "#4F81BD" if n in TECH or n.endswith("_CCS") else
1230.                 "#C0504D" if n.endswith("_Procurement") else
1231.                 "#9BBB59"
1232.                 for n in nodes
1233.             ],
1234.             hovertemplate="%{label}"
1235.         ),
1236.         link=dict(
1237.             source=[idx[s] for s, _, _ in flows],
1238.             target=[idx[d] for _, d, _ in flows],
1239.             value = [v / scale for _, v in flows],
1240.             color="rgba(160,160,160,0.35)",
1241.             hovertemplate=(
1242.                 "%{source.label} → %{target.label}"
1243.                 "<br>{%value:.2f} "+unit
1244.             )
1245.         )
1246.     )
1247. )
1248.
1249. fig.update_layout(
1250.     title=dict(
1251.         text=f"Material flows – {t} ({mode})",
1252.         x=0.5, xanchor="center"
1253.     ),
1254.     font=dict(size=11)
1255. )
1256.
1257. if outfile is None:
1258.     outfile = f"sankey_{mode}_{t}.html"
1259. fig.write_html(outfile, include_plotlyjs="cdn")
1260. print(f"☑ Sankey written to {outfile}")
1261.
1262. # — example run – comment out if you prefer not to auto-generate
1263. if __name__ == "__main__":
1264.     for mode in ("material", "energy", "combined"):
1265.         sankey_year(2030, mode=mode, top_n=40, min_flow=0.5)

```

Annex 3 Parameters excel file

Macroeconomic parameters																				
WACC		8%																		
Inflation		2.0%		real_WACC		5.9%														
Demand										Import prices										
(t / year)		(t / year)		(t / year)		(t / year)		(t / year)		(€/ t)		(€/ t)		(€/ t)		(€/ t)		(€/ t)		
PP		PS		PET		PVC		PUR		PE (HD/LD/LL)		PP		PS		PET		PVC		
2025	647,000	238,000	207,000	445,000	214,000	936,000	224,000	976,000	230,000	1,000	830	2,340	1,250	1,150	1,771	1,380	1,079	1,625	1,938	
2030	673,000	259,000	225,000	483,000	233,000	1,017,000	235,000	1,093,000	2035	1,200	955	2,670	638	1,380	2,002	1,300	1,079	1,625	1,938	
2040	733,000	270,000	234,000	504,000	243,000	1,060,000	2040	1,656	2,125	1,380	1,145	3,229	1,725	1,380	2,125	1,380	1,145	3,229	1,725	
2045	764,000	281,000	244,000	525,000	253,000	1,105,000	2045	1,758	2,256	1,465	1,216	3,428	1,831	1,465	2,256	1,465	1,216	3,428	1,831	
2050	797,000	293,000	254,000	547,000	264,000	1,152,000	2050	1,860	2,387	1,550	1,287	3,627	1,938	1,550	2,387	1,550	1,287	3,627	1,938	
Feedstock prices										Feedstock price multipliers										
(€/t)		(€/t)		(€/t)		(€/GJ)		(€/GJ)		(€/t)		(€/t)		(€/t)		(€/t)		(€/t)		
Naphtha		Propane		Ethane		Natural Gas		Steam		Hydrogen		Propylene		Ethylene		Benzene		p-Xylene		
2025	585	490	215	11.4	11.4	33.3	900	1,035	1,093	1,208	989	863	753	2,670	638	1,380	1,079	1,625	1,938	
2030	673	564	247	11	10.8	29	1,035	1,093	1,208	989	863	753	2,670	638	1,380	1,079	1,625	1,938	1,938	
2035	761	637	280	10	10.3	24	1,170	1,235	1,365	1,118	975	852	2,340	722	1,380	1,079	1,625	1,938	1,938	
2040	807	676	297	10	10.3	19	1,242	1,311	1,449	1,187	1,035	904	2,010	766	1,380	1,079	1,625	1,938	1,938	
2045	857	718	315	10	10.3	15	1,319	1,392	1,538	1,260	1,099	960	1,680	813	1,380	1,079	1,625	1,938	1,938	
2050	907	760	333	10	10.3	10	1,395	1,473	1,628	1,333	1,163	1,015	1,350	860	1,380	1,079	1,625	1,938	1,938	
Electricity and carbon prices																				
(€/GJ)		(€/t CO2)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		(€/t CO2 / GJ)		
Electricity price		Carbon price		Grid emissions		Grid emission factors		Natural Gas emission factors		Hydrogen emission factor										
2025	21.0	42.8	100%	0.12	0.06	0	2030	21.0	43.9	80%	0.10	0.06	0	2035	21.0	43.9	60%	0.07	0.06	0
2040	21.0	44.2	40%	0.05	0.06	0	2045	21.0	44.4	20%	0.02	0.06	0	2050	21.0	44.7	0%	0.00	0.06	0
2050	21.0	44.7	0%	0.00	0.06	0														
Decarbonization levers parameters										Capacity expansion parameters										
Learning curve (% / 5-years)		Ecracker		H2		CCS		Eboiler		Steam cracker (A)		Steam cracker (B)		Catalytic reforming		PP		PS		
Fixed OPEX (% of CAPEX)				12%		6%		7%		5%		5%		5%		6%		2%		
		0%		0%		0%		0%		3%		4%		5%		2%		2%		
		3%		4%		5%		2%												
Decarbonization levers (CAPEX)										Capacity expansion (CAPEX)										
Ecracker (€/t of ethylene · y)		H2 (€/GJ · y)		CCS (€/t of CO2 · y)		Eboiler (€/GJ · y)				Steam cracker (A) (€/t of ethylene · y)		Steam cracker (B) (€/t of ethylene · y)		Catalytic reforming (€/t of reformate · y)		PP (€/t of PP · y)		PS (€/t of PS · y)		
2025	400	2.0	70	3.0	2030	352	1.9	65	2.9	2035	310	1.8	61	2.7	2040	273	1.7	56	2.6	
2045	240	1.6	52	2.4	2050	211	1.5	49	2.3	2025	1,600	1,600	2,200	650	800	600	750	1,100	800	
														</						

Type		Propylene	Ethylene	Benzene	p-Xylene	Toluene	Epoxy	Electricity	Steam	Hydrogen	Natural Gas	CO2 (reaction)	CO2 (energy)	CO2 (electricity)	CO2 (fuel)	PP	PS	PET	PVC	PUR	PE (HD/LD/LL)	Ethane	Propane	n-Butane	Naphtha	Aromatics	Butadiene	C4/C5+FO	CH ₄ / fuel-gas	Reformate	VGO	
Base	Steam cracking A_base	0.116	0.503		0.01	0.011	0.013	0	-0.02	0	0	-2.06	0	1.05	0.0042	1.0458	0	0	0	0	0	-0.349	-0.185	-0.045	-0.415	0.049	0.038	0.117	0.017	0	0	
Increment	Steam cracking A_Ecracker	0	0	0	0	0	0	0	-2.06	0	0	2.06	0	0	-1.0458	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Increment	Steam cracking A_CCS	0	0	0	0	0	0	0	0	0	0	0	-1.05	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Base	Steam cracking B	0.116	0.503		0.01	0	0	0	-0.051	0	0	-3.67	0	1.03	0.01071	1.01929	0	0	0	0	0	-0.349	-0.185	-0.045	-0.415	0.049	0.038	0.117	0.017	0	0	
Increment	Steam cracking B_Ecracker	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Increment	Steam cracking B_CCS	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Base	Catalytic reforming	0	0	0.0341496	0.1440342	0.1282446		0	-0.24	0	0	-1.46	0	0.123	0.0504	0.0726	0	0	0	0	0	0	0	0	-1	0	0	0	0.017	0.918	0	0
Increment	Catalytic reforming_H2	0	0	0	0	0	0	0	0	0	-1.46	1.46	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	Catalytic reforming_CCS	0	0	0	0	0	0	0	0	0	0	0	-0.123	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	
Base	HDA	0	0	1	0	-1.1		0	-0.21	-1.1	0	-2.86	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Propylene FCC	1.1	0	0	0	0	0	0	-0.6	0.65	0	-5.35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	-5.35	0
Base	PP	-1	0	0	0	0	0	0	-1.15	-0.8	0	0	0.02	0.3	0.2415	0.0585	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PP_Eboiler	0	0	0	0	0	0	0	-0.8	0.8	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PP_H2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PP_CCS	0	0	0	0	0	0	0	0	0	0	0	-0.02	-0.3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	PS	0	-0.278	-0.773	0	0	0	0	-0.66	-3.1	0	-4.72	0.08	0.74	0.1386	0.6014	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PS_Eboiler	0	0	0	0	0	0	0	-3.1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PS_H2	0	0	0	0	0	0	0	0	0	-4.72	4.72	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PS_CCS	0	0	0	0	0	0	0	0	0	0	0	-0.08	-0.74	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	PET	0	-0.23	0	-0.64	0		0	-2.59	-6.38	0	-3.35	0.36	1.31	0.5439	0.7661	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PET_Eboiler	0	0	0	0	0	0	0	-6.38	6.38	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PET_H2	0	0	0	0	0	0	0	0	0	-3.35	3.35	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PET_CCS	0	0	0	0	0	0	0	0	0	-0.36	0	0	-1.31	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	PVC	0	-0.45	0	0	0	0	0	-1.3	-2.31	0	-3.6	0.11	0.65	0.273	0.377	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PVC_Eboiler	0	0	0	0	0	0	0	-2.31	2.31	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PVC_H2	0	0	0	0	0	0	0	0	0	-3.6	3.6	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PVC_CCS	0	0	0	0	0	0	0	0	0	0	0	-0.11	-0.65	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	PUR	0	0	0	0	-0.062	-0.83	-1.84	-1.77	0	-1.98	0.04	0.57	0.3864	0.1836	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0
Increment	PUR_Eboiler	0	0	0	0	0	0	-1.77	1.77	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PUR_H2	0	0	0	0	0	0	0	0	-1.98	1.98	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PUR_CCS	0	0	0	0	0	0	0	0	0	0	-0.04	-0.57	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	PE (HD/LD/LL)	0	-1	0	0	0		0	-2.04	-0.64	0	0.03	0.47	0.4284	0.0416	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
Increment	PE (HD/LD/LL)_Eboiler	0	0	0	0	0	0	-0.64	0.64	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PE (HD/LD/LL)_H2	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Increment	PE (HD/LD/LL)_CCS	0	0	0	0	0	0	0	0	0	0	-0.03	-0.47	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PP	0	0	0	0	0	0	0	0	0	0	-1.1	0	0.32	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PS	0	0	0	0	0	0	0	0	0	0	0	2.91	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PET	0	0	0	0	0	0	0	0	0	0	-15	0	0.9	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PVC	0	0	0	0	0	0	0	0	0	0	-25.7	0	1.94	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PUR	0	0	0	0	0	0	0	0	0	0	-5	0	4.7	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
Base	Recycling PE (HD/LD/LL)	0	0	0	0	0	0	0	0	0	0	-6.4	0	0.4	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Naphtha_Procurement	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0
PROC	n-Butane_Procurement	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0
PROC	Propane_Procurement	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0
PROC	Ethane_Procurement	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0
PROC	Natural Gas_Procurement	0	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Steam_Procurement	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Hydrogen_Procurement	0	0	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Electricity_Procurement	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Propylene_Procurement	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Ethylene_Procurement	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Benzene_Procurement	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	p-Xylene_Procurement	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Toluene_Procurement	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	Epoxy_Procurement	0	0	0	0	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
PROC	VGO_Procurement	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

Annex 4 Model results tables

year	polymer	produced	demand
	PE		
2025	(HD/LD/LL)	936,000	936,000
2025	PET	207,000	207,000
2025	PP	647,000	647,000
2025	PS	238,000	238,000
2025	PUR	214,000	214,000
2025	PVC	445,000	445,000
	PE		
2030	(HD/LD/LL)	976,000	976,000
2030	PET	215,000	215,000
2030	PP	675,000	675,000
2030	PS	248,000	248,000
2030	PUR	224,000	224,000
2030	PVC	463,000	463,000
	PE		
2035	(HD/LD/LL)	1,017,000	1,017,000
2035	PET	225,000	225,000
2035	PP	703,000	703,000
2035	PS	259,000	259,000
2035	PUR	233,000	233,000
2035	PVC	483,000	483,000
	PE		
2040	(HD/LD/LL)	1,060,000	1,060,000
2040	PET	234,000	234,000
2040	PP	733,000	733,000
2040	PS	270,000	270,000
2040	PUR	243,000	243,000
2040	PVC	504,000	504,000
	PE		
2045	(HD/LD/LL)	1,105,000	1,105,000
2045	PET	244,000	244,000
2045	PP	764,000	764,000
2045	PS	281,000	281,000
2045	PUR	253,000	253,000
2045	PVC	525,000	525,000
	PE		
2050	(HD/LD/LL)	1,152,000	1,152,000
2050	PET	254,000	254,000
2050	PP	797,000	797,000
2050	PS	293,000	293,000
2050	PUR	264,000	264,000

2050 PVC 547,000 547,000

year	comm	net
2025	Ethylene	0
2025	Electricity	0
2025	Steam	0
	Natural	
2025	Gas	0
2025	Naphtha	0
2025	n-Butane	0
2025	Propane	0
2025	Ethane	0
2025	Benzene	0
2025	p-Xylene	28,507
2025	Toluene	0
2025	Propylene	0
2025	Hydrogen	0
2025	Epoxy	0
2030	Ethylene	0
2030	Electricity	0
2030	Steam	0
	Natural	
2030	Gas	0
2030	Naphtha	0
2030	n-Butane	0
2030	Propane	0
2030	Ethane	0
2030	Benzene	0
2030	p-Xylene	30,193
2030	Toluene	0
2030	Propylene	0
2030	Hydrogen	0
2030	Epoxy	0
2035	Ethylene	0
2035	Electricity	0
2035	Steam	0
	Natural	
2035	Gas	0
2035	Naphtha	0
2035	n-Butane	0
2035	Propane	0
2035	Ethane	0

2035	Benzene	0
2035	p-Xylene	31,241
2035	Toluene	0
2035	Propylene	0
2035	Hydrogen	0
2035	Epoxy	0
2040	Ethylene	0
2040	Electricity	0
2040	Steam	0
	Natural	
2040	Gas	0
2040	Naphtha	0
2040	n-Butane	0
2040	Propane	0
2040	Ethane	0
2040	Benzene	0
2040	p-Xylene	32,930
2040	Toluene	0
2040	Propylene	0
2040	Hydrogen	0
2040	Epoxy	0
2045	Ethylene	0
2045	Electricity	0
2045	Steam	0
	Natural	
2045	Gas	0
2045	Naphtha	0
2045	n-Butane	0
2045	Propane	0
2045	Ethane	0
2045	Benzene	0
2045	p-Xylene	33,936
2045	Toluene	0
2045	Propylene	0
2045	Hydrogen	0
2045	Epoxy	0
2050	Ethylene	0
2050	Electricity	0
2050	Steam	0
	Natural	
2050	Gas	0
2050	Naphtha	0
2050	n-Butane	0

2050	Propane	0
2050	Ethane	0
2050	Benzene	0
2050	p-Xylene	35,672
2050	Toluene	0
2050	Propylene	0
2050	Hydrogen	0
2050	Epoxy	0

Year	icity_Procure	ky_Procure	ne_Procure	ne_Procure	gen_Procure	lha_Procure	al_Gas_Procure	ne_Procure	m_Procure	m_Procure	O_Procure	m_Procure	ne_Procure	ne_Procure
2025	4,813,790	177,620	867,313	0	1,959,243	12,425,830	459,750	4,510,035	1,793,620	111,831				
2030	5,017,989	185,920	903,892	0	2,041,986	12,949,968	479,140	4,695,870	1,872,830	116,548				
2035	5,231,696	193,390	942,301	0	2,130,962	13,506,176	499,501	4,902,054	1,948,998	121,500				
2040	5,453,147	201,690	982,251	1,472,965	2,221,444	12,607,410	520,678	5,107,903	2,032,606	126,651				
2045	5,682,614	209,990	1,023,748	2,780,756	2,313,124	11,887,661	542,675	5,321,900	2,118,642	132,002				
2050	5,924,352	219,120	1,067,138	5,038,875	2,411,712	10,254,124	565,675	5,545,763	2,211,533	137,597				

year	tech	P	Cap
2025	Steam cracking A_base	2,485,137	2,485,137
	Steam cracking		
2025	A_Ecracker	0	0
2025	Catalytic reforming	927,911	1,000,000
2025	Catalytic reforming_H2	0	0
2025	Catalytic reforming_CCS	0	0
2025	PE (HD/LD/LL)	936,000	936,000
2025	PE (HD/LD/LL)_Eboiler	0	0
2025	PE (HD/LD/LL)_H2	0	0
2025	PE (HD/LD/LL)_CCS	0	0
2025	PP	647,000	647,000
2025	PP_Eboiler	0	0
2025	PP_H2	0	0
2025	PP_CCS	0	0
2025	PVC	445,000	445,000
2025	PVC_Eboiler	0	0
2025	PVC_H2	0	0
2025	PVC_CCS	22,250	22,250
2025	PUR	214,000	214,000
2025	PUR_Eboiler	0	0
2025	PUR_H2	0	0
2025	PUR_CCS	0	0
2025	PS	238,000	238,000
2025	PS_Eboiler	0	0
2025	PS_H2	0	0
2025	PS_CCS	11,900	11,900
2025	PET	207,000	207,000
2025	PET_Eboiler	0	0
2025	PET_H2	0	0
2025	PET_CCS	10,350	10,350
2025	HDA	127,435	127,435
2025	Propylene FCC	326,113	326,113
2030	Steam cracking A_base	2,589,948	2,589,948
	Steam cracking		
2030	A_Ecracker	0	0
2030	Catalytic reforming	967,158	1,000,000
2030	Catalytic reforming_H2	0	0
2030	Catalytic reforming_CCS	0	0
2030	PE (HD/LD/LL)	976,000	976,000
2030	PE (HD/LD/LL)_Eboiler	0	0
2030	PE (HD/LD/LL)_H2	0	0
2030	PE (HD/LD/LL)_CCS	0	0

2030	PP	675,000	675,000
2030	PP_Eboiler	0	0
2030	PP_H2	0	0
2030	PP_CCS	0	0
2030	PVC	463,000	463,000
2030	PVC_Eboiler	0	0
2030	PVC_H2	0	0
2030	PVC_CCS	46,300	46,300
2030	PUR	224,000	224,000
2030	PUR_Eboiler	0	0
2030	PUR_H2	0	0
2030	PUR_CCS	0	0
2030	PS	248,000	248,000
2030	PS_Eboiler	0	0
2030	PS_H2	0	0
2030	PS_CCS	24,800	24,800
2030	PET	215,000	215,000
2030	PET_Eboiler	0	0
2030	PET_H2	0	0
2030	PET_CCS	21,500	21,500
2030	HDA	132,776	132,776
2030	Propylene FCC	340,515	340,515
2035	Steam cracking A_base	2,700,004	2,700,004
	Steam cracking		
2035	A_Ecracker	0	0
2035	Catalytic reforming	1,010,460	1,010,460
2035	Catalytic reforming_H2	0	0
2035	Catalytic reforming_CCS	0	0
2035	PE (HD/LD/LL)	1,017,000	1,017,000
2035	PE (HD/LD/LL)_Eboiler	0	0
2035	PE (HD/LD/LL)_H2	0	0
2035	PE (HD/LD/LL)_CCS	0	0
2035	PP	703,000	703,000
2035	PP_Eboiler	0	0
2035	PP_H2	0	0
2035	PP_CCS	0	0
2035	PVC	483,000	483,000
2035	PVC_Eboiler	0	0
2035	PVC_H2	0	0
2035	PVC_CCS	72,450	72,450
2035	PUR	233,000	233,000
2035	PUR_Eboiler	0	0
2035	PUR_H2	0	0

2035	PUR_CCS	34,950	34,950
2035	PS	259,000	259,000
2035	PS_Eboiler	0	0
2035	PS_H2	0	0
2035	PS_CCS	38,850	38,850
2035	PET	225,000	225,000
2035	PET_Eboiler	0	0
2035	PET_H2	0	0
2035	PET_CCS	33,750	33,750
2035	HDA	138,700	138,700
2035	Propylene FCC	354,363	354,363
2040	Steam cracking A_base	2,814,473	2,814,473
	Steam cracking		
2040	A_Ecracker	0	0
2040	Catalytic reforming	1,053,438	1,053,438
2040	Catalytic reforming_H2	263,359	263,359
2040	Catalytic reforming_CCS	0	0
2040	PE (HD/LD/LL)	1,060,000	1,060,000
2040	PE (HD/LD/LL)_Eboiler	0	0
2040	PE (HD/LD/LL)_H2	0	0
2040	PE (HD/LD/LL)_CCS	318,000	318,000
2040	PP	733,000	733,000
2040	PP_Eboiler	0	0
2040	PP_H2	0	0
2040	PP_CCS	0	0
2040	PVC	504,000	504,000
2040	PVC_Eboiler	0	0
2040	PVC_H2	126,000	126,000
2040	PVC_CCS	151,200	151,200
2040	PUR	243,000	243,000
2040	PUR_Eboiler	0	0
2040	PUR_H2	60,750	60,750
2040	PUR_CCS	72,900	72,900
2040	PS	270,000	270,000
2040	PS_Eboiler	0	0
2040	PS_H2	67,500	67,500
2040	PS_CCS	81,000	81,000
2040	PET	234,000	234,000
2040	PET_Eboiler	0	0
2040	PET_H2	58,500	58,500
2040	PET_CCS	70,200	70,200
2040	HDA	144,591	144,591
2040	Propylene FCC	369,565	369,565

2045	Steam cracking A_base	2,933,376	2,933,376
	Steam cracking		
2045	A_Ecracker	0	0
2045	Catalytic reforming	1,095,773	1,095,773
2045	Catalytic reforming_H2	438,309	438,309
2045	Catalytic reforming_CCS	0	0
2045	PE (HD/LD/LL)	1,105,000	1,105,000
2045	PE (HD/LD/LL)_Eboiler	0	0
2045	PE (HD/LD/LL)_H2	0	0
2045	PE (HD/LD/LL)_CCS	552,500	552,500
2045	PP	764,000	764,000
2045	PP_Eboiler	0	0
2045	PP_H2	0	0
2045	PP_CCS	0	0
2045	PVC	525,000	525,000
2045	PVC_Eboiler	0	0
2045	PVC_H2	210,000	210,000
2045	PVC_CCS	262,500	262,500
2045	PUR	253,000	253,000
2045	PUR_Eboiler	0	0
2045	PUR_H2	101,200	101,200
2045	PUR_CCS	126,500	126,500
2045	PS	281,000	281,000
2045	PS_Eboiler	0	0
2045	PS_H2	112,400	112,400
2045	PS_CCS	140,500	140,500
2045	PET	244,000	488,000
2045	PET_Eboiler	0	0
2045	PET_H2	195,200	195,200
2045	PET_CCS	244,000	244,000
2045	HDA	150,459	150,459
2045	Propylene FCC	385,208	385,208
2050	Steam cracking A_base	3,057,702	3,057,702
	Steam cracking		
2050	A_Ecracker	0	0
2050	Catalytic reforming	1,142,766	1,142,766
2050	Catalytic reforming_H2	685,660	685,660
2050	Catalytic reforming_CCS	0	0
2050	PE (HD/LD/LL)	1,152,000	1,152,000
2050	PE (HD/LD/LL)_Eboiler	0	0
2050	PE (HD/LD/LL)_H2	0	0
2050	PE (HD/LD/LL)_CCS	806,400	806,400
2050	PP	797,000	797,000

2050	PP_Eboiler	0	0
2050	PP_H2	0	0
2050	PP_CCS	557,900	557,900
2050	PVC	547,000	781,429
2050	PVC_Eboiler	0	0
2050	PVC_H2	468,857	468,857
2050	PVC_CCS	547,000	547,000
2050	PUR	264,000	264,000
2050	PUR_Eboiler	0	0
2050	PUR_H2	158,400	158,400
2050	PUR_CCS	184,800	184,800
2050	PS	293,000	418,571
2050	PS_Eboiler	0	0
2050	PS_H2	251,143	251,143
2050	PS_CCS	293,000	293,000
2050	PET	254,000	488,000
2050	PET_Eboiler	0	0
2050	PET_H2	254,000	254,000
2050	PET_CCS	254,000	254,000
2050	HDA	156,887	156,887
2050	Propylene FCC	402,097	402,097

year	tech	capacity_adde d	unit_cape x	total_capex	annuity_cape x
2025	HDA	127,435	280	35,681,757	1,795,128
2025	PET_CCS	10,350	70	724,500	36,449
2025	PS_CCS	11,900	70	833,000	41,908
2025	PVC_CCS	22,250	70	1,557,500	78,357
2025	Propylene FCC Steam cracking	326,113	280	91,311,586	4,593,831
2025	A_base	485,137	1,600	776,219,483	39,051,135
2030	HDA	5,342	274	1,465,739	73,740
2030	PE (HD/LD/LL)	40,000	784	31,360,000	1,577,703
2030	PET	8,000	588	4,704,000	236,655
2030	PET_CCS	11,150	65	725,865	36,518
2030	PP	28,000	637	17,836,000	897,318
2030	PS	10,000	784	7,840,000	394,426
2030	PS_CCS	12,900	65	839,790	42,249
2030	PUR	10,000	1,078	10,780,000	542,335
2030	PVC	18,000	735	13,230,000	665,593
2030	PVC_CCS	24,050	65	1,565,655	78,767
2030	Propylene FCC	14,402	274	3,951,836	198,814

	Steam cracking				
2030	A_base	104,811	1,520	159,312,922	8,014,937
2035	Catalytic reforming	10,460	1,944	20,334,350	1,023,009
2035	HDA	5,924	269	1,592,948	80,140
2035	PE (HD/LD/LL)	41,000	768	31,501,120	1,584,802
2035	PET	10,000	576	5,762,400	289,903
2035	PET_CCS	12,250	61	741,652	37,312
2035	PP	28,000	624	17,479,280	879,372
2035	PS	11,000	768	8,451,520	425,191
2035	PS_CCS	14,050	61	850,629	42,795
2035	PUR	9,000	1,056	9,507,960	478,340
2035	PUR_CCS	34,950	61	2,115,978	106,454
2035	PVC	20,000	720	14,406,000	724,757
2035	PVC_CCS	26,150	61	1,583,199	79,650
2035	Propylene FCC	13,849	269	3,724,075	187,356
	Steam cracking				
2035	A_base	110,056	1,444	158,920,382	7,995,189
2040	Catalytic reforming	42,977	1,827	78,531,872	3,950,891
	Catalytic				
2040	reforming_H2	263,359	2	437,484	22,010
2040	HDA	5,891	264	1,552,385	78,100
2040	PE (HD/LD/LL)	43,000	753	32,377,005	1,628,868
2040	PE (HD/LD/LL)_CCS	318,000	56	17,904,987	900,789
2040	PET	9,000	565	5,082,437	255,694
2040	PET_CCS	36,450	56	2,052,317	103,251
2040	PET_H2	58,500	2	97,178	4,889
2040	PP	30,000	612	18,353,244	923,341
2040	PS	11,000	753	8,282,490	416,687
2040	PS_CCS	42,150	56	2,373,255	119,397
2040	PS_H2	67,500	2	112,129	5,641
2040	PUR	10,000	1,035	10,353,112	520,859
2040	PUR_CCS	37,950	56	2,136,774	107,500
2040	PUR_H2	60,750	2	100,916	5,077
2040	PVC	21,000	706	14,823,774	745,775
2040	PVC_CCS	78,750	56	4,434,018	223,073
2040	PVC_H2	126,000	2	209,307	10,530
2040	Propylene FCC	15,201	264	4,006,090	201,544
	Steam cracking				
2040	A_base	114,469	1,372	157,028,828	7,900,026
2045	Catalytic reforming	42,336	1,718	72,717,726	3,658,385
	Catalytic				
2045	reforming_H2	174,950	2	273,184	13,744
2045	HDA	5,868	258	1,515,547	76,246
2045	PE (HD/LD/LL)	45,000	738	33,205,254	1,670,536

2045	PE (HD/LD/LL)_CCS	234,500	52	12,279,274	617,763
2045	PET	254,000	553	140,568,908	7,071,937
2045	PET_CCS	173,800	52	9,100,801	457,856
2045	PET_H2	136,700	2	213,457	10,739
2045	PP	31,000	600	18,585,718	935,036
2045	PS	11,000	738	8,116,840	408,353
2045	PS_CCS	59,500	52	3,115,637	156,746
2045	PS_H2	44,900	2	70,111	3,527
2045	PUR	10,000	1,015	10,146,050	510,442
2045	PUR_CCS	53,600	52	2,806,691	141,203
2045	PUR_H2	40,450	2	63,163	3,178
2045	PVC	21,000	692	14,527,299	730,860
2045	PVC_CCS	111,300	52	5,828,073	293,207
2045	PVC_H2	84,000	2	131,166	6,599
2045	Propylene FCC	15,643	258	4,040,009	203,250
	Steam cracking				
2045	A_base	118,903	1,303	154,955,037	7,795,695
2050	Catalytic reforming	46,992	1,615	75,873,450	3,817,148
	Catalytic				
2050	reforming_H2	247,350	1	363,063	18,265
2050	HDA	6,428	253	1,626,904	81,849
2050	PE (HD/LD/LL)	47,000	723	33,987,422	1,709,887
2050	PE (HD/LD/LL)_CCS	253,900	49	12,364,469	622,049
2050	PET_CCS	10,000	49	486,982	24,500
2050	PET_H2	58,800	1	86,307	4,342
2050	PP	33,000	588	19,389,101	975,454
2050	PP_CCS	557,900	49	27,168,718	1,366,842
2050	PS	137,571	723	99,482,940	5,004,927
2050	PS_CCS	152,500	49	7,426,473	373,621
2050	PS_H2	138,743	1	203,648	10,245
2050	PUR	11,000	994	10,937,442	550,256
2050	PUR_CCS	58,300	49	2,839,104	142,834
2050	PUR_H2	57,200	1	83,959	4,224
2050	PVC	256,429	678	173,843,339	8,745,954
2050	PVC_CCS	284,500	49	13,854,634	697,018
2050	PVC_H2	258,857	1	379,953	19,115
2050	Propylene FCC	16,889	253	4,274,633	215,054
	Steam cracking				
2050	A_base	124,326	1,238	153,921,796	7,743,713

year	family	Fam_year	installed_cap_tpa
2025	CCS	CCS2025	44,500

2025	Eboiler	Eboiler2025	0
2025	Ecracker	Ecracker2025	0
2025	H2	H22025	0
2030	CCS	CCS2030	92,600
2030	Eboiler	Eboiler2030	0
2030	Ecracker	Ecracker2030	0
2030	H2	H22030	0
2035	CCS	CCS2035	180,000
2035	Eboiler	Eboiler2035	0
2035	Ecracker	Ecracker2035	0
2035	H2	H22035	0
2040	CCS	CCS2040	693,300
2040	Eboiler	Eboiler2040	0
2040	Ecracker	Ecracker2040	0
2040	H2	H22040	576,109
2045	CCS	CCS2045	1,326,000
2045	Eboiler	Eboiler2045	0
2045	Ecracker	Ecracker2045	0
2045	H2	H22045	1,057,109
2050	CCS	CCS2050	2,643,100
2050	Eboiler	Eboiler2050	0
2050	Ecracker	Ecracker2050	0
2050	H2	H22050	1,818,060

Year	feed_raw_cost	feed_energy_cost	capex_annuity	fom_cost	direct_CO2_cost	elec_CO2_cost	fuel_CO2_cost	steam_CO2_cost	Total_CO2_cost	total_cost
2025	3,159,475,701	398,992,109	326,817,542	273,044,201	13,169,472	41,471,766	53,083,144	19,266,870	126,991,252	4,285,320,805
2030	3,646,758,984	411,583,683	339,576,600	266,356,237	25,913,020	68,003,782	108,779,727	39,445,305	242,141,835	4,906,417,338
2035	4,164,343,750	418,993,585	353,510,869	261,232,400	33,140,610	68,367,798	145,866,702	52,942,184	300,317,293	5,498,397,898
2040	4,513,537,575	451,547,864	371,634,810	260,522,211	32,107,100	54,106,129	108,549,797	43,979,043	238,742,069	5,835,984,529
2045	4,896,483,259	470,352,869	350,803,303	262,444,683	17,562,840	31,354,392	81,311,603	36,401,796	166,630,631	6,146,714,746
2050	5,310,051,909	477,834,712	370,171,543	268,306,555	4,579,500	0	46,143,559	24,955,932	75,678,991	6,502,043,710

year	tech	installed_cap	unit_opex_eur_per_tpa	opex_cost_eur
2025	Catalytic reforming	1,000,000	110	110,000,000
2025	HDA	127,435	6	713,635
2025	PE (HD/LD/LL)	936,000	16	14,976,000
2025	PET	207,000	12	2,484,000
2025	PET_CCS	10,350	4	36,225
2025	PP	647,000	13	8,411,000
2025	PS	238,000	16	3,808,000
2025	PS_CCS	11,900	4	41,650
2025	PUR	214,000	22	4,708,000
2025	PVC	445,000	15	6,675,000
2025	PVC_CCS	22,250	4	77,875
2025	Propylene FCC	326,113	6	1,826,232
	Steam cracking			
2025	A_base	2,485,137	48	119,286,584
2030	Catalytic reforming	1,000,000	103	103,400,000
2030	HDA	132,776	5	728,677
2030	PE (HD/LD/LL)	976,000	16	15,303,680
2030	PET	215,000	12	2,528,400
2030	PET_CCS	21,500	3	69,983
2030	PP	675,000	13	8,599,500
2030	PS	248,000	16	3,888,640
2030	PS_CCS	24,800	3	80,724
2030	PUR	224,000	22	4,829,440
2030	PVC	463,000	15	6,806,100
2030	PVC_CCS	46,300	3	150,707
2030	Propylene FCC	340,515	5	1,868,744
	Steam cracking			
2030	A_base	2,589,948	46	118,101,643
2035	Catalytic reforming	1,010,460	97	98,212,718
2035	HDA	138,700	5	745,963
2035	PE (HD/LD/LL)	1,017,000	15	15,627,629
2035	PET	225,000	12	2,593,080
2035	PET_CCS	33,750	3	102,166
2035	PP	703,000	12	8,777,096
2035	PS	259,000	15	3,979,898
2035	PS_CCS	38,850	3	117,605
2035	PUR	233,000	21	4,923,010
2035	PUR_CCS	34,950	3	105,799
2035	PVC	483,000	14	6,958,098
2035	PVC_CCS	72,450	3	219,317
2035	Propylene FCC	354,363	5	1,905,850

	Steam cracking			
2035	A_base	2,700,004	43	116,964,172
2040	Catalytic reforming	1,053,438	91	96,246,548
	Catalytic			
2040	reforming_H2	263,359	0	0
2040	HDA	144,591	5	762,091
2040	PE (HD/LD/LL)	1,060,000	15	15,962,616
2040	PE (HD/LD/LL)_CCS	318,000	3	895,249
2040	PET	234,000	11	2,642,867
2040	PET_CCS	70,200	3	197,631
2040	PET_H2	58,500	0	0
2040	PP	733,000	12	8,968,619
2040	PS	270,000	15	4,065,949
2040	PS_CCS	81,000	3	228,035
2040	PS_H2	67,500	0	0
2040	PUR	243,000	21	5,031,612
2040	PUR_CCS	72,900	3	205,232
2040	PUR_H2	60,750	0	0
2040	PVC	504,000	14	7,115,412
2040	PVC_CCS	151,200	3	425,666
2040	PVC_H2	126,000	0	0
2040	Propylene FCC	369,565	5	1,947,855
	Steam cracking			
2040	A_base	2,814,473	41	115,826,828
2045	Catalytic reforming	1,095,773	86	94,107,641
	Catalytic			
2045	reforming_H2	438,309	0	0
2045	HDA	150,459	5	777,160
2045	PE (HD/LD/LL)	1,105,000	15	16,307,469
2045	PE (HD/LD/LL)_CCS	552,500	3	1,446,546
2045	PET	488,000	11	5,401,388
2045	PET_CCS	244,000	3	638,836
2045	PET_H2	195,200	0	0
2045	PP	764,000	12	9,160,961
2045	PS	281,000	15	4,146,967
2045	PS_CCS	140,500	3	367,855
2045	PS_H2	112,400	0	0
2045	PUR	253,000	20	5,133,901
2045	PUR_CCS	126,500	3	331,200
2045	PUR_H2	101,200	0	0
2045	PVC	525,000	14	7,263,649
2045	PVC_CCS	262,500	3	687,273
2045	PVC_H2	210,000	0	0

2045	Propylene FCC Steam cracking	385,208	5	1,989,698
2045	A_base	2,933,376	39	114,684,138
2050	Catalytic reforming Catalytic	1,142,766	81	92,254,855
2050	reforming_H2	685,660	0	0
2050	HDA	156,887	5	794,155
2050	PE (HD/LD/LL)	1,152,000	14	16,661,068
2050	PE (HD/LD/LL)_CCS	806,400	2	1,963,511
2050	PET	488,000	11	5,293,360
2050	PET_CCS	254,000	2	618,467
2050	PET_H2	254,000	0	0
2050	PP	797,000	12	9,365,523
2050	PP_CCS	557,900	2	1,358,436
2050	PS	418,571	14	6,053,687
2050	PS_CCS	293,000	2	713,428
2050	PS_H2	251,143	0	0
2050	PUR	264,000	20	5,249,972
2050	PUR_CCS	184,800	2	449,971
2050	PUR_H2	158,400	0	0
2050	PVC	781,429	14	10,595,243
2050	PVC_CCS	547,000	2	1,331,895
2050	PVC_H2	468,857	0	0
2050	Propylene FCC Steam cracking	402,097	5	2,035,397
2050	A_base	3,057,702	37	113,567,585

year	polymer	family	incremental_cost_€/t
	PE		
2025	(HD/LD/LL)	CCS	6.12
	PE		
2025	(HD/LD/LL)	Eboiler	25.77
	PE		
2025	(HD/LD/LL)	H2	0.12
2025	PET	CCS	-18.61
2025	PET	Eboiler	255.33
2025	PET	H2	73.48
2025	PP	CCS	6.84
2025	PP	Eboiler	32.17
2025	PP	H2	0.12
2025	PS	CCS	1.33
2025	PS	Eboiler	124.16

2025	PS	H2	103.49
2025	PUR	CCS	5.41
2025	PUR	Eboiler	70.97
2025	PUR	H2	43.48
2025	PVC	CCS	-0.81
2025	PVC	Eboiler	92.56
2025	PVC	H2	78.96
2025	—	Ecracker	200.76
	PE		
2030	(HD/LD/LL)	CCS	3.48
	PE		
2030	(HD/LD/LL)	Eboiler	29.99
	PE		
2030	(HD/LD/LL)	H2	0.11
2030	PET	CCS	-43.87
2030	PET	Eboiler	297.46
2030	PET	H2	59.72
2030	PP	CCS	4.88
2030	PP	Eboiler	37.45
2030	PP	H2	0.11
2030	PS	CCS	-4.67
2030	PS	Eboiler	144.62
2030	PS	H2	84.10
2030	PUR	CCS	2.08
2030	PUR	Eboiler	82.65
2030	PUR	H2	35.34
2030	PVC	CCS	-8.87
2030	PVC	Eboiler	107.81
2030	PVC	H2	64.17
2030	—	Ecracker	200.16
	PE		
2035	(HD/LD/LL)	CCS	1.74
	PE		
2035	(HD/LD/LL)	Eboiler	30.03
	PE		
2035	(HD/LD/LL)	H2	0.10
2035	PET	CCS	-58.73
2035	PET	Eboiler	297.91
2035	PET	H2	45.96
2035	PP	CCS	3.54
2035	PP	Eboiler	37.50
2035	PP	H2	0.10
2035	PS	CCS	-8.33
2035	PS	Eboiler	144.83

2035	PS	H2	64.71
2035	PUR	CCS	-1.13
2035	PUR	Eboiler	82.76
2035	PUR	H2	27.21
2035	PVC	CCS	-13.73
2035	PVC	Eboiler	107.97
2035	PVC	H2	49.38
2035	—	Ecracker	187.81
	PE		
2040	(HD/LD/LL)	CCS	-0.50
	PE		
2040	(HD/LD/LL)	Eboiler	28.18
	PE		
2040	(HD/LD/LL)	H2	0.10
2040	PET	CCS	-68.15
2040	PET	Eboiler	279.60
2040	PET	H2	30.32
2040	PP	CCS	2.54
2040	PP	Eboiler	35.19
2040	PP	H2	0.10
2040	PS	CCS	-10.75
2040	PS	Eboiler	135.93
2040	PS	H2	42.69
2040	PUR	CCS	-2.55
2040	PUR	Eboiler	77.68
2040	PUR	H2	17.96
2040	PVC	CCS	-16.90
2040	PVC	Eboiler	101.33
2040	PVC	H2	32.58
2040	—	Ecracker	170.90
	PE		
2045	(HD/LD/LL)	CCS	-1.59
	PE		
2045	(HD/LD/LL)	Eboiler	25.54
	PE		
2045	(HD/LD/LL)	H2	0.09
2045	PET	CCS	-76.83
2045	PET	Eboiler	253.27
2045	PET	H2	14.70
2045	PP	CCS	1.62
2045	PP	Eboiler	31.88
2045	PP	H2	0.09
2045	PS	CCS	-12.99
2045	PS	Eboiler	123.13

2045	PS	H2	20.68
2045	PUR	CCS	-3.87
2045	PUR	Eboiler	70.37
2045	PUR	H2	8.72
2045	PVC	CCS	-19.83
2045	PVC	Eboiler	91.79
2045	PVC	H2	15.79
2045	—	Ecracker	152.72
	PE		
2050	(HD/LD/LL)	CCS	-2.62
	PE		
2050	(HD/LD/LL)	Eboiler	22.18
	PE		
2050	(HD/LD/LL)	H2	0.09
2050	PET	CCS	-85.12
2050	PET	Eboiler	219.83
2050	PET	H2	-0.92
2050	PP	CCS	-0.12
2050	PP	Eboiler	27.68
2050	PP	H2	0.09
2050	PS	CCS	-15.12
2050	PS	Eboiler	106.88
2050	PS	H2	-1.33
2050	PUR	CCS	-5.12
2050	PUR	Eboiler	61.09
2050	PUR	H2	-0.52
2050	PVC	CCS	-22.62
2050	PVC	Eboiler	79.68
2050	PVC	H2	-1.00
2050	—	Ecracker	133.41