Supplementary Information for

Climate Impact of Primary Plastic Production

Nihan Karali, Nina Khanna, and Nihar Shah

Lawrence Berkeley National Laboratory
** Corresponding author. Email: NKarali@lbl.gov*

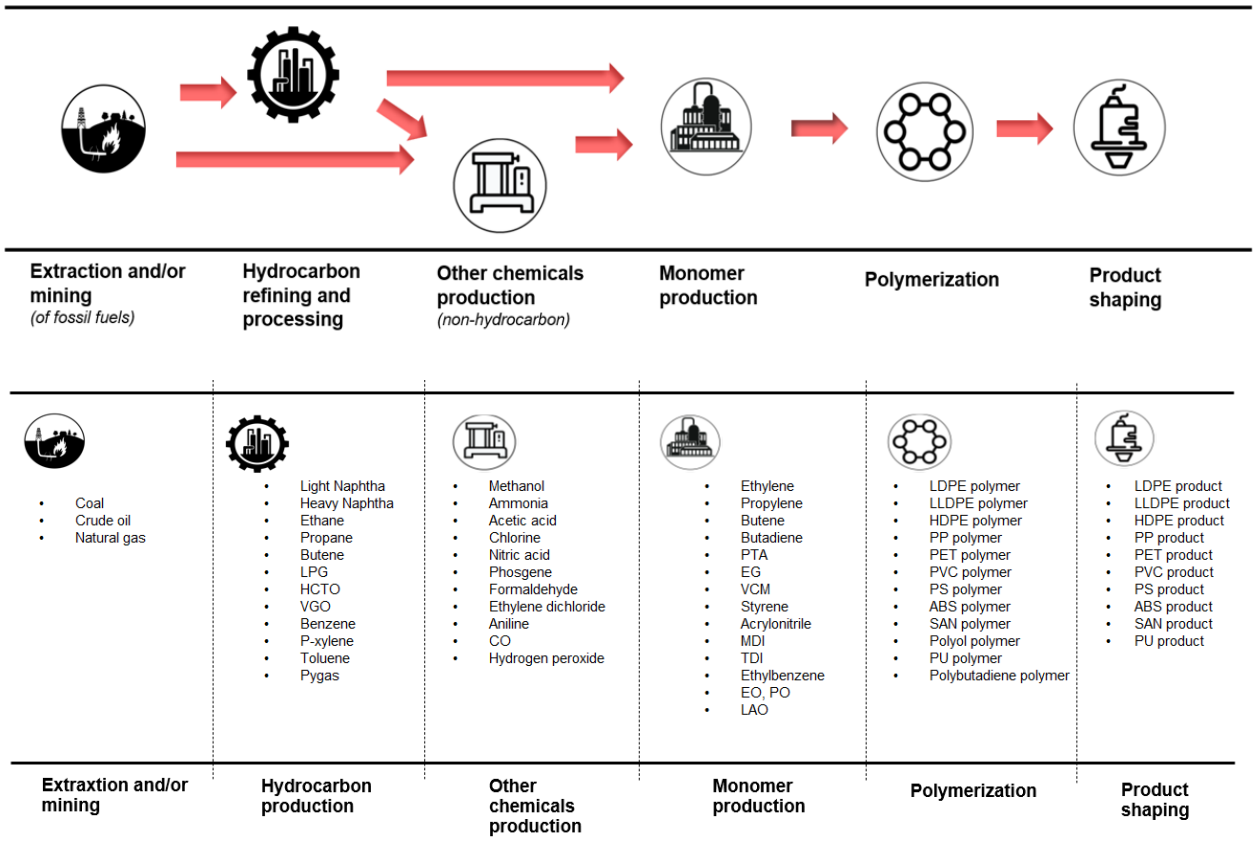
Global Primary Plastic Production (GPPP) model

The GPPP model is a bottom-up, technology-resolved framework that tracks input coefficients, fuel-disaggregated energy consumption, and direct process emissions through fossil-fuel extraction, hydrocarbon refining, non-hydrocarbon chemicals production, monomer production, polymerization, and product manufacturing. In the model, production is defined as equal to demand; through material-flow links, production then determines activity and the associated energy consumption and emissions at each technology node.

Mathematical framework

This section presents the mathematical framework (developed on Microsoft Excel) used to model primary plastic production in a bottom-up approach. The framework tracks material and energy flows across six distinct production stages, from fossil fuel extraction through final product shaping, as illustrated in Supplementary Fig. S23. By explicitly modeling intermediate products—including fossil fuels, hydrocarbons, chemicals, monomers, and polymers—this approach enables detailed quantification of energy consumption and greenhouse gas (GHG) emissions at each production stage.

The model includes the production value chain of common plastic polymers: low-density polyethylene (LDPE), linear low-density polyethylene (LLDPE), high-density polyethylene (HDPE), polypropylene (PP), polyethylene terephthalate (PET), polyvinyl chloride (PVC), polystyrene (PS), acrylonitrile butadiene styrene (ABS), and polyurethane (PU). Each technology node is defined by input coefficients (input requirements per unit output), energy consumption (energy combustion per unit output) disaggregated by fuel type, and direct process emissions (carbon monoxide (CO), carbon dioxide (CO_2), nitrogen oxides (NO_x), sulfur oxides (SO_x), and other process chemical gases). Total GHG emissions are calculated as the sum of combustion of energy-related CO_2 and process emissions, converted to CO_2 equivalent (CO_2e).



Supplementary Fig. S1. Production stages of primary plastics with material details

Notes: *(1) A hydrocarbon is a chemical compound consisting entirely of hydrogen and carbon. (2) A polymer is a large molecule that is made out of many smaller molecules that are joined together by covalent bonds. The smaller, repeating molecules are called monomers. (3) Ethylene dichloride (EDC) is a chlorinated hydrocarbon, in which chlorine substituted for hydrogen. Since EDC does not contain hydrogen and is not always a direct refinery output, it is considered under the "Other chemicals production" step in our modeling. (4) Benzene is a trimer, but, the trimerization is a chemical reaction, not a fundamental property of benzene itself. Benzene's molecular structure meet the specific definition of a hydrocarbon. CO = carbon monoxide, EG = ethylene glycol, EO = ethylene oxide, HCTO = hydrocracker tail oil, HDPE = high-density polyethylene, LAO = linear alpha olefins, LDPE = low-density polyethylene, LLDPE = linear low-density polyethylene, LPG = liquid petroleum gas, MDI = methylene diphenyl diisocyanate, PET = polyethylene terephthalate, PO = propylene oxide, Polyol = polyolefins, PP = polypropylene, PS = polystyrene, PTA = purified terephthalic acid, PU = polyurethane, PVC = polyvinyl chloride, P-xylene = paraxylene, Pygas = pyrolysis gasoline, SAN = styrene acrylonitrile, TDI = toluene diisocyanate, VCM = vinyl chloride monomer, VGO = vacuum gas oil.*

The framework uses a mass allocation criterion when modeling material output from production systems with multiple outputs. This approach, known as "coproduct allocation," distributes energy consumption and emissions across multiple product lines. The ratio of the mass of each coproduct over the total mass output is used to allocate emissions, allowing us to associate GHG emissions to products based on mass production volume. While coproduct allocation can be performed using different criteria (including stoichiometric, elemental, reaction enthalpy, and

economic allocation), mass allocation is most appropriate for our framework's material flow tracking approach.

The modeling equations below describe mass balance constraints, technology shares, and emission calculations for each production stage. The framework explicitly tracks material flows from extraction to finished products, handles both single-output and multiproduct technologies, and separately accounts for fossil fuels as feedstock versus process energy. For comprehensive descriptions of primary plastic production pathways, technology options, and detailed input data for each polymer type, please refer to the main report.

Plastic production modeling equations

a) Product shaping

The modeling framework establishes mass balance constraints to ensure production meets demand. Eq. 1 constrains total production of each finished plastic product to equal its corresponding demand, while Eq. 2 distributes this production across different shaping technologies according to their market shares.

$$PP_{p,t} = D_{p,t} \quad \text{(Eq.1)}$$

$$PP_{m,p,t} = PP_{p,t} * \alpha 1_{m,p,t}, m \in m_{pp} \quad \text{(Eq.2)}$$

where:

$D_{p,t}$: Total demand for plastic product p in year t
$PP_{p,t}$: Total production of plastic product p in year t
$PP_{m,p,t}$: Production of plastic product p from product shaping technology m in year t
$\alpha 1_{m,p,t}$: Share of product shaping technology m used in production of product p in year t (e.g., 70% of LDPE products come from film extrusion in 2020)
p: Plastic product by polymer type (LDPE product, LLDPE product, HDPE product, PP product, PVC product, PS product, ABS product, PU product)
m: technology type
m_{pp}: Set of product shaping technologies (injection molding, blow molding, rotational molding, film extrusion, other extrusion, fibers, sheets, profiles, tubes, pipes and fittings, others)

Energy consumption and associated GHG emissions from product shaping are calculated in Eq.s 3-6. Eq. 3 determines energy use based on production volume and technology-specific energy intensity, Eq. 4 disaggregates this energy by fuel type, Eq. 5 aggregates total energy across all technologies, and Eq. 6 converts fuel consumption to emissions using fuel-specific emission factors.

$$E_{m,p,t} = PP_{m,p,t} * \in_{m,p}, m \in m_{pp} \quad \text{(Eq.3)}$$

$$E_{m,p,t} = \sum_e E_{m,p,t} * e_{share_{m,e}}, m \in m_{pp} \quad \text{(Eq.4)}$$

$$E_{p,t} = \sum_{m \in m_{pp}} E_{m,p,t} \quad \text{(Eq.5)}$$

$$Emis_{p,t} = \sum_{e} \sum_{m \in m_{pp}} E_{m,p,t} * e_{share_{m,e}} * e_{factor_e} \quad \text{(Eq.6)}$$

where:

$E_{m,p,t}$: Energy consumption for production of finished plastic product p using product shaping technology m in year t

$E_{p,t}$: Total energy consumption for the shaping of all finished plastic products p in year t

$Emis_{p,t}$: Total GHG emissions from the shaping of all finished plastic product ps in year t

$\in_{m,p}$: Energy intensity of technology $m \in m_{pp}$ for product shaping of finished plastic product p *(e.g., GJ/tonne)*

$e_{share_{m,e}}$: Share of fuel type e in total energy used in technology m

e_{factor_e}: CO_2 emission factor for combustion of fuel type e *(e.g., $kgCO_2/GJ$)*,

e: Fuel type (electricity, natural gas, heating oil, refinery oil, coal, etc).

Note: Demand projections ($D_{p,t}$) are exogenous inputs rather than endogenous model outputs. Section C.2.4.2 provides the global plastic demand by polymer type from 2019 to 2050 based on OECD projections *(57)*. For detailed definitions and data on production shares and energy intensities of product shaping technologies, refer to the main report.

b) <u>Polymerization</u>

Polymer production must satisfy the input requirements of all product shaping technologies. Eq. 7 calculates total polymer demand by aggregating the polymer inputs needed across all shaping processes, accounting for material losses during product fabrication. Eq. 8 allocates polymer production across different polymerization technologies based on their market shares.

$$P_{p,t} = \sum_{m \in m_{pp}} PP_{m,p,t} * \beta 1_{m,p} \quad \text{(Eq.7)}$$

$$P_{m,p,t} = P_{p,t} * \alpha 2_{m,p,t}\ , m \in m_p \quad \text{(Eq.8)}$$

where:

$P_{p,t}$: Total production of polymer p used in shaping of plastic product p in year t

$P_{m,p,t}$: Production of polymer p from polymerization technology m in year t

$\beta 1_{m,p}$: Polymer p input coefficient to product shaping technology $m \in m_{pp}$ per unit of finished product p (accounts for polymer loss during shaping of plastic products)

$\alpha 2_{m,p,t}$: Share of polymerization technology m used in production of polymer p in year t (e.g., polymerization processes for general-purpose polystyrene (GPPS) and suspension polymerization for EPS. Similarly, bottle-grade PETs require solid-state polymerization on top of regular polymerization of PET)

p: Polymer type (LDPE polymer, LLDPE polymer, HDPE polymer, PP polymer, PVC polymer, PS polymer, ABS polymer, PU polymer)

m_p: Set of polymerization technologies

Energy consumption and GHG emissions from polymerization are calculated in Eq.s 9-12. These equations follow the same structure as product shaping but include an additional term in Eq. 12 for process emissions that occur independently of fuel combustion (e.g., emissions from chemical reactions during polymerization).

$$E_{m,p,t} = P_{m,p,t} * \in_{m,p} \ldots\ldots\ldots\ldots, m \in m_p \quad \text{(Eq.9)}$$

$$E_{m,p,t} = \sum_e E_{m,p,t} * e_{share_{m,e}}, m \in m_p \quad \text{(Eq.10)}$$

$$E_{p,t} = \sum_{m \in m_p} E_{m,p,t} \quad \text{(Eq.11)}$$

$$Emis_{p,t} = \sum_e \sum_{m \in m_p} E_{m,p,t} * e_{share_{m,e}} * e_{factor_e} + \sum_o P_{m,p,t} * e_{process_{m,o}} \quad \text{(Eq.12)}$$

where:

$E_{m,p,t}$: Energy consumption for polymerization of polymer p using polymerization technology m in year t

$E_{p,t}$: Total energy consumption for polymerization of polymer p in year t (if more than one technology is used as in the case with PS)

$Emis_{p,t}$: Total GHG emissions from polymerization of polymer p in year t

$\in_{m,p}$: Energy intensity of technology $m \in m_p$ used for polymerization of polymer p

$e_{share_{m,e}}$: share of fuel type e in total energy used in technology m

e_{factor_e}: CO2 emission factor for combustion of fuel type e

$e_{process_{m,o}}$: process emission factor of GHG gas o for technology m

e: Fuel type (electricity, natural gas, heating oil, refinery oil, coal, etc)

Note: For detailed definitions of polymerization technologies, processes, and polymer-specific data, refer to the main report.

c) Monomer production

Total monomer production from various technologies must satisfy the input requirements of all polymerization processes. Monomers are produced through multiple pathways including steam cracking, methanol-to-olefins (MTO), fluid catalytic cracking (FCC), propane dehydrogenation (PDH), purified terephthalic acid (PTA) production, and styrene production, among others.

Eq. 13 calculates the total demand for each monomer required to produce a specific polymer by summing the monomer inputs across all polymerization technologies. Eq.s 14-16 track monomer flows from production technologies through to specific polymer applications, enabling allocation of environmental impacts across the full production chain.

$$M_{i,p,t} = \sum_{m \in m_p} P_{m,p,t} * \beta 2_{m,i,p} \quad \text{(Eq.13)}$$

$$M_{m,i,p,t} = M_{i,p,t} * \alpha 3_{m,i,t}, m \in m_i \quad \text{(Eq.14)}$$

$$M_{m,i,t} = \sum_p M_{m,i,p,t} \quad \text{(Eq.15)}$$

$$M_{i,t} = \sum_{m \in m_i} M_{m,i,t} \quad \text{(Eq.16)}$$

where:

$M_{i,p,t}$: Production of monomer i used in polymerization of polymer p in year t
$M_{m,i,p,t}$: Production of monomer i by monomer production technology $m \in m_i$ for use in polymerization of polymer p in year t
$M_{m,i,t}$: Production of monomer i by monomer production technology $m \in m_i$ in year t
$M_{i,t}$: Total production of monomer i used in polymerization of all polymers included in the modeling in year t,
$\beta 2_{m,i,p}$: Monomer i input coefficient to polymerization technology $m \in m_p$ per unit of polymer p,
$\alpha 3_{m,i,t}$: Share of monomer production technology $m \in m_i$ used in production of monomer i in year t (e.g., in 2019, ethylene was produced via 36% light naphtha steam cracking, 39% ethane steam cracking, 16% light hydrocarbon gas mix steam cracking, with smaller contributions from HCTO (0.5%), VGO (5%), and MTO (3.5%))
i: Monomer type (ethylene, propylene, butadiene, PTA, EG, VCM, styrene, acrylonitrile, MDI, TDI, benzene, ethylbenzene, EO, PO, LAO)
m_p: Set of polymerization technologies
m_i: Set of monomer production technologies (steam cracking, MTO, FCC, PDH, Metathesis and Superflex, PTA production, EG production, VCM production, styrene production, acrylonitrile production, TDI production, MDI production, EO production, PO production)

Energy consumption and GHG emissions from monomer production are calculated using a similar approach to previous stages. A key complexity in monomer production is that many technologies, particularly steam cracking, operate as multiproduct processes that simultaneously generate multiple high-value products from a single feedstock input. Not all of these outputs are monomers. For example, steam cracking of light naphtha yields not just monomers (ethylene, propylene, butadiene), but also valuable hydrocarbons such as benzene, xylene, and toluene (collectively BTX) and pyrolysis gas (pygas). BTX and pygas play significant roles in the PET production value chain. To account for these multiproduct outputs, we use the term "high-value products" (hvp) to encompass both monomers and valuable hydrocarbon co-products. Eq.s 17-21 handle the allocation of energy and emissions across these co-products.

$$E_{m,hvp,t} = M_{m,i,t} * \in_{m,hvp}, m \in m_i \quad \text{(Eq.17)}$$

$$E_{m,hvp,p,t} = M_{m,i,p,t} * \in_{m,hvp}, m \in m_i \quad \text{(Eq.18)}$$

$$E_{m,hvp,p,t} = \sum_e E_{m,hvp,p,t} * e_{share_{m,e}}, m \in m_i \quad \text{(Eq.19)}$$

$$E_{hvp,p,t} = \sum_{m \in m_i} E_{m,hvp,p,t} \quad \text{(Eq.20)}$$

$$Emis_{hvp,p,t} = \sum_e \sum_{m \in m_i} E_{m,hvp,p,t} * e_{share_{m,e}} * e_{factor_e} + \sum_o M_{m,hvp,p,t} * e_{process_{m,o}} \quad \text{(Eq.21)}$$

where:

$E_{m,hvp,t}$: Energy consumption for production of high-value-product hvp by monomer production technology $m \in m_i$ in year t

$E_{m,hvp,p,t}$: Energy consumption for production of high-value-product hvp by monomer production technology $m \in m_i$ for use in polymerization of polymer p in year t

$E_{hvp,p,t}$: Total energy consumption for production of high-value-product hvp for use in polymerization of polymer p in year t

$Emis_{hvp,p,t}$: Total GHG emissions from production of high-value-product hvp for polymer p in year t

$\in_{m,hvp}$: Energy intensity of technology $m \in m_i$ used for production of high-value-product hvp

hvp: High-value product type. In some technologies (e.g., MTO), high-value products consist only of monomers ($hvp \equiv i$). In contrast, steam cracking technologies generate both monomers and valuable hydrocarbon co-products (e.g., BTX, pygas), all of which are included in the hvp set.

$e_{share_{m,e}}$: share of fuel type e in total energy used in technology m

e_{factor_e}: CO2 emission factor for combustion of fuel type e

$e_{process_{m,o}}$: process emission factor of GHG gas o for technology m

e: Fuel types (electricity, natural gas, heating oil, refinery oil, coal, etc).

Note: For detailed definitions of monomer production technologies, process descriptions, and monomer-specific data, refer to the main report.

d) Hydrocarbon refining and processing

Hydrocarbons serve as the fundamental building blocks for monomer production and must be supplied through refining and processing of fossil fuel feedstocks. Similar to monomer production, many hydrocarbon refining processes operate as multiproduct facilities that simultaneously generate multiple hydrocarbon outputs from a single feedstock. Total hydrocarbon production must satisfy the input requirements of all monomer production technologies.

Some hydrocarbons used in monomer production technologies generating only single output (e.g., propane dehydrogenation generates monomer propylene), thus tracking hydrocarbon allocation for the output monomer from these technologies is easier. However, allocation of hydrocarbon use for monomers from monomer production technologies that simultaneously generate multiple outputs (e.g., steam crackers) it is more complex.

The complexity of hydrocarbon allocation depends on the structure of the downstream monomer production technology. Monomer production technologies can be categorized into two types:

Single-output technologies ($m_{\,i\ subset\ 1}$): These produce only one monomer from hydrocarbon inputs (e.g., propane dehydrogenation generates only propylene). Hydrocarbon allocation for these technologies is straightforward.

Multi-output technologies ($m_{\,i\ subset\ 2}\}$): These simultaneously generate multiple high-value products from hydrocarbon inputs (e.g., steam crackers produce monomers plus BTX and pygas). Hydrocarbon allocation for these technologies requires a more sophisticated mass-balance approach.

Hydrocarbon demand from single-output monomer production technologies

Eq.s 22-24 calculate hydrocarbon demand for monomer production technologies that generate a single output (a monomer), where allocation is straightforward.

$$HC_{h,i,t} = \sum_{m \in m_{i\ subset\ 1}} M_{m,i,t} * \beta 3_{m,h,i} \quad \text{(Eq.22)}$$

$$HC_{h,i,p,t} = \sum_{m \in m_{i\ subset\ 1}} M_{m,i,p,t} * \beta 3_{m,h,i} \quad \text{(Eq.23)}$$

$$HC_{m,h,i,t} = HC_{h,i,t} * \alpha 4_{m,h,t}, m \in m_h \quad \text{(Eq.24)}$$

where:

$HC_{h,i,t}$: Total demand for hydrocarbon h for the production of monomer i in year t
$HC_{h,i,p,t}$: Total demand for hydrocarbon h for the production of monomer i for use in polymerization of polymer p in year t
$HC_{m,h,i,t}$: Production of hydrocarbon h for the production of monomer i in year t
$\beta 3_{m,h,i}$: Hydrocarbon h input coefficient to monomer production technology $m \in m_{i\ subset\ 1}$ per unit of monomer i
$\alpha 4_{m,h,t}$: Share of hydrocarbon production technology $m \in m_h$ used in production of hydrocarbon h in year t
$m_{\,i\ subset\ 1}$: Subset of monomer production technologies $m \in m_i$ that generate single product
m_h: Set of hydrocarbon production technologies
h: Hydrocarbon type (light naphtha, heavy naphtha, ethane, propane, butane, LPG, HCTO, VGO, p-xylene, toluene, benzene, pygas)

Hydrocarbon demand from multi-output monomer production technologies

Eq.s 25-34 calculate hydrocarbon demand for multi-output monomer production technologies and allocate production across their various outputs, tracking material flows from specific hydrocarbons through to their eventual use in particular polymers. The allocation methodology follows a mass-balance approach similar to that used in the fossil fuel extraction stage.

First, Eq. 25 identifies the theoretical hydrocarbon demand for each individual high-value product, calculated as if that product were produced independently rather than as part of a multiproduct operation.

$$HC\ tdemand_{h,hvp,t} = M_{m,hvp,t} * \beta 3_{m,h,hvp}, m \in m_{i\ subset\ 2} \quad \text{(Eq.25)}$$

where:

$HC\ tdemand_{h,hvp,t}$: Theoretical demand for hydrocarbon h for production of high-value-product hvp in year t

$\beta 3_{m,h,hvp}$: Hydrocarbon h input coefficient to monomer production technology $m \in m_{i\ subset\ 2}$ per unit of high-value-product hvp

$m_{i\ subset\ 2}$: subset of monomer production technologies $m \in m_i$ that generate multiproduct

Eq.s 26-27 determine the actual hydrocarbon demand from multi-output technologies by taking the maximum theoretical demand across all high-value products (ensuring sufficient hydrocarbon supply for all outputs) and verifying that this hydrocarbon level can indeed produce the required quantities of each high-value product. The balance constraint in Eq. 27 must be non-negative, confirming that hydrocarbon supply meets or exceeds demand for each product.

$$HC_{h,hvp,t} = \max\left(HC\ tdemand_{h,hvp,t}\right) \quad \text{(Eq.26)}$$

$$M\ balance_{m,i,t} = \frac{HC_{h,hvp,t}}{\beta 3_{m,h,hvp}} - M_{m,hvp,t} \geq 0 \quad for\ each\ hvp, m \in m_{i\ subset\ 2} \quad \text{(Eq.27)}$$

where:

$HC_{h,hvp,t}$: Demand for hydrocarbon h for production of high-value-product hvp in year t

$M\ balance_{m,i,t}$: Balance check ensuring sufficient hydrocarbon h to produce high-value product hvp from technology $m \in m_{i\ subset\ 2}$ in year t

$\beta 3_{m,h,hvp}$: Hydrocarbon h input coefficient to monomer production technology $m \in m_{i\ subset\ 2}$ per unit of high-value-product hvp

After establishing sufficient hydrocarbon availability for all high-value products from multi-output technologies ($m \in m_{i\ subset\ 2}$), Eq.s 28-34 calculate total hydrocarbon production requirements and allocate these flows across polymers, enabling tracking of hydrocarbon use from refining through final products.

$$HC_{h,t} = \sum_{hvp} M_{m,hvp,t} * \beta 3_{m,h,hvp}, m \in m_{i\ subset\ 2} \quad \text{(Eq.28)}$$

$$HC_{h,hvp,t} = M_{m,hvp,t} * \beta 3_{m,h,hvp}, m \in m_{i\ subset\ 2} \quad \text{(Eq.29)}$$

$$HC_{h,hvp,p,t} = M_{m,hvp,p,t} * \beta 3_{m,h,hvp}, m \in m_{i\ subset\ 2} \quad \text{(Eq.30)}$$

$$HC_{h,p,t} = \sum_{hvp} HC_{h,hvp,p,t} \quad \text{(Eq.31)}$$

$$HC_{m,h,t} = HC_{h,t} * \alpha 4_{m,h,t}, m \in m_h \quad \text{(Eq.32)}$$

$$HC_{m,h,hvp,t} = HC_{h,hvp,t} * \alpha 4_{m,h,t}, m \in m_h \quad \text{(Eq.33)}$$

$$HC_{m,h,hvp,p,t} = HC_{h,hvp,p,t} * \alpha 4_{m,h,t}, m \in m_h \quad \text{(Eq.34)}$$

where:

$HC_{h,t}$: Total demand of hydrocarbon h in year t
$HC_{h,hpv,t}$: Demand of hydrocarbon h for high-value product hvp in year t
$HC_{h,hpv,p,t}$: Demand of hydrocarbon h for high-value product hvp to be used in production of polymer p in year t
$HC_{h,p,t}$: Total demand of hydrocarbon h for polymer p in year t,
$HC_{m,h,t}$: Production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ in year t
$HC_{m,h,hvp,t}$: Production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ for use in production of high-value product hvp in year t
$HC_{m,h,hvp,p,t}$: Production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ for use in production of high-value product hvp and subsequently in polymer p in year t

Energy consumption and GHG emissions from hydrocarbon refining and processing are calculated in Eq.s 35-42, following the same methodological approach as previous production stages. An important note: energy consumption and GHG emissions from hydrocarbons produced as co-products within monomer production technologies (e.g., BTX and pygas produced by steam cracking) are accounted for in the monomer production stage, not here, to avoid double-counting.

The energy intensity parameters ($\in_{m,h}$) encompass all refining and processing steps required to produce each hydrocarbon. For example, light naphtha from crude oil distillation undergoes hydrotreating for purification before entering steam cracking; both the distillation and hydrotreating energy requirements are captured in the energy intensity parameter.

$$E_{m,h,t} = HC_{m,h,t} * \in_{m,h}, m \in m_h \quad \text{(Eq.35)}$$

$$E_{m,h,i\ or\ hvp,t} = HC_{m,h,i\ or\ hvp,t} * \in_{m,h}, m \in m_h \quad \text{(Eq.36)}$$

$$E_{m,h,i\ or\ hvp,p,t} = HC_{m,h,i\ or\ hvp,p,t} * \in_{m,h}, m \in m_h \quad \text{(Eq.37)}$$

$$E_{m,h,t} = \sum_e E_{h,m,t} * e_{share_{m,e}}, m \in m_h \quad \text{(Eq.38)}$$

$$E_{m,h,i\ or\ hvp,t} = \sum_e E_{m,h,i\ or\ hvp,t} * e_{share_{m,e}}, m \in m_h \quad \text{(Eq.39)}$$

$$E_{m,h,i\ or\ hvp,p,t} = \sum_e E_{m,h,i\ or\ hvp,p,t} * e_{share_{m,e}}, m \in m_h \quad \text{(Eq.40)}$$

$$E_{h,i\ or\ hvp,p,t} = \sum_{m \in m_h} E_{m,h,i\ or\ hvp,p,t} \quad \text{(Eq.41)}$$

$$Emis_{h,i\ or\ hvp,p,t} = \sum_e \sum_{m \in m_h} E_{m,h,i\ or\ hvp,p,t} * e_{share}{}_{m,e} * e_{factor}{}_e + \sum_o HC_{m,h,i\ or\ hvp,p,t} * e_{process}{}_{m,o} \quad \text{(Eq.42)}$$

where:

$E_{m,h,t}$: Energy consumption for production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ in year t

$E_{m,h,i\ or\ hvp,t}$: Energy consumption for production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ for use in production of monomer i or high-value product hvp in year t

$E_{m,h,i\ or\ hvp,p,t}$: Energy consumption for production of hydrocarbon h by hydrocarbon production technology $m \in m_h$ for use in production of monomer i or high-value product hvp and subsequently in polymerization of polymer p in year t

$E_{h,i\ or\ hvp,p,t}$: Total energy consumption for production of hydrocarbon h for use in production of monomer i or high-value product hvp and subsequently for polymerization of polymer p in year t

$Emis_{h,i\ or\ hvp,p,t}$: Total GHG emissions from production of hydrocarbon h for monomer i or high-value product hvp and subsequently for polymer p in year t,

$\in_{m,h}$: Energy intensity of technology $m \in m_h$ used for production of hydrocarbon h

$e_{share}{}_{m,e}$: share of fuel type e in total energy used in technology m,

$e_{factor}{}_e$: CO2 emission factor for combustion of fuel type e

$e_{process}{}_{m,o}$: process emission factor of GHG gas o for technology m

e: Fuel types (electricity, natural gas, heating oil, refinery oil, coal, etc)

Note: For detailed definitions of hydrocarbon production technologies and hydrocarbon-specific data, refer to the main report.

e) <u>Non-hydrocarbon chemicals production</u>

While hydrocarbons provide the carbon backbone for most plastic monomers, certain monomer production processes require additional non-hydrocarbon chemicals as reactants or catalysts. For example, vinyl chloride monomer (VCM) production requires chlorine, and purified terephthalic acid (PTA) production requires acetic acid as a solvent and catalyst. These chemicals encompass a diverse range of inorganic and organic compounds including oxidizers (chlorine, nitric acid, hydrogen peroxide), acids (acetic acid), bases (ammonia), and various organic intermediates.

Total production of these non-hydrocarbon chemicals must satisfy the input requirements of their respective monomer production technologies. Eq.s 43-47 calculate chemical demand for each monomer and track material flows through to final polymer applications, maintaining the allocation chain established in previous stages.

$$C_{c,i,t} = \sum_{m \in m_i} M_{m,i,t} * \beta 4_{m,c,i} \quad \text{(Eq.43)}$$

$$C_{c,i,p,t} = \sum_{m \in m_i} M_{m,i,p,t} * \beta 4_{m,c,i} \quad \text{(Eq.44)}$$

$$C_{m,c,i,t} = C_{c,i,t} * \alpha 5_{m,c,t}\ , m \in m_c \quad \text{(Eq.45)}$$

$$C_{m,c,t} = \sum_i C_{m,c,i,t} \quad \text{(Eq.46)}$$

$$C_{c,t} = \sum_{m \in m_c} C_{m,c,t} \quad \text{(Eq.47)}$$

where:

$C_{c,i,t}$: Total demand for chemical c for the production of monomer i in year t
$C_{c,i,p,t}$: Total demand for chemical c for the production of monomer i for use in polymerization of polymer p in year t
$C_{m,c,i,t}$: Production of chemical c by chemical production technology $m \in m_c$ for the production of monomer i in year t
$C_{m,c,t}$: Production of chemical c by chemical production technology $m \in m_c$ in year t
$C_{c,t}$: Total production of chemical c used in the model in year t
$\beta 4_{m,c,i}$: Chemical c input coefficient to monomer production technology $m \in m_i$ per unit of monomer i
$\alpha 5_{m,c,t}$: Share of chemical production technology $m \in m_c$ used in production of chemical c in year t (e.g., in 2019, chlorine was produced via 59% membrane technology, 29% mercury process, and 12% diaphragm process)
c: Chemical type (methanol, ammonia, acetic acid, chlorine, nitric acid, phosgene, formaldehyde, EDC, aniline, CO, hydrogen peroxide)
m_c: Set of chemical production technologies

Energy consumption and GHG emissions from chemical production are calculated in Eq.s 48-52. These equations follow the structure established in previous stages, tracking energy use and emissions through to specific polymer products to enable full supply chain allocation.

$$E_{m,c,i,t} = C_{m,c,i,t} * \in_{m,c},\ m \in m_c \quad \text{(Eq.48)}$$

$$E_{m,c,i,t} = \sum_e E_{m,c,i,t} * e_{share}{}_{m,e},\ m \in m_c \quad \text{(Eq.49)}$$

$$E_{c,i,t} = \sum_{m \in m_c} E_{m,c,i,t} \quad \text{(Eq.50)}$$

$$Emis_{c,i,t} = \sum_e \sum_{m \in m_{mc}} E_{m,c,i,t} * e_{share}{}_{m,e} * e_{factor}{}_e + \sum_o C_{m,c,t} * e_{process}{}_{m,o} \quad \text{(Eq.51)}$$

where:

$E_{m,c,i,t}$: Energy consumption for production of chemical c using chemical production technology $m \in m_c$ for use in production of monomer i in year t
$E_{c,i,t}$: Total energy consumption for production of chemical c for use in production of monomer i in year t
$Emis_{c,i,t}$: Total GHG emissions from production of chemical c for monomer i in year t
$\in_{m,c}$: Energy intensity of technology $m \in m_c$ used for the production of chemical c
$e_{share}{}_{m,e}$: share of fuel type e in total energy used in technology m

e_{factor_e}: CO2 emission factor for combustion of fuel type e

$e_{process_{m,o}}$: process emission factor of GHG gas o for technology m

e: Fuel types (electricity, natural gas, heating oil, refinery oil, coal, etc).

Note: For detailed definitions of chemical production technologies, processes, and chemical-specific data, refer to the main report.

f) Fossil fuel extraction/mining

Fossil fuels, namely crude oil, natural gas, and coal, are used as both feedstock and energy sources for process heat throughout the production chain. The extraction and processing of these fossil fuels encompasses multiple activities including exploration, drilling, fracking, mining, production, surface processing, and transportation to refineries or processing facilities. Each activity generates emissions through direct sources (such as methane (CH_4) leakage and flaring) and indirect sources (fuel combustion during extraction operations).

Feedstock demand

Hydrocarbon refineries and processing facilities operate as multiproduct production systems, similar to the steam crackers described in earlier stages. The framework employs a mass-balance allocation approach to ensure sufficient fossil fuel feedstock is available to produce all required hydrocarbons while properly accounting for the co-product nature of these facilities.

Eq. 52 calculates the theoretical fossil fuel feedstock demand for producing a single hydrocarbon product, assuming it were produced in isolation rather than as part of a multiproduct operation.

$$F\ tdemand_{f,h,t} = \sum_i HC_{m,h,t} * \beta 5_{m,f,h},\ m \in m_h \qquad \text{(Eq.52)}$$

where:

$F\ tdemand_{f,h,t}$: Theoretical demand for fossil fuel f for production of hydrocarbon h in year t

$\beta 5_{m,f,h}$: Fossil fuel f input coefficient to hydrocarbon production technology $m \in m_h$ per unit of hydrocarbon h

m_h: Set of hydrocarbon production technologies

Eq.s 53-54 determine the actual fossil fuel demand from multiproduct hydrocarbon production facilities by taking the maximum theoretical demand across all hydrocarbon products (ensuring sufficient feedstock for all outputs) and verifying that this feedstock level can indeed produce the required quantities of each hydrocarbon. The balance in Eq. 55 must be non-negative, confirming fossil fuel supply meets or exceeds demand for each hydrocarbon product.

$$F_{f,h,t} = \max\left(F\ tdemand_{f,h,t}\right) \qquad \text{(Eq.53)}$$

$$HC\ balance_{m,h,t} = \frac{F_{f,h,t}}{\beta 5_{m,f,h}} - HC_{m,h,t} \geq 0 \qquad for\ each\ h, m \in m_h \qquad \text{(Eq.54)}$$

where:

$F_{f,h,t}$: Demand of fossil fuel f for production of hydrocarbon h in year t

$HC\ balance_{m,h,t}$: Balance check ensuring sufficient fossil fuel f to produce hydrocarbon h from technology $m \in m_h$ in year t

$\beta 5_{m,f,h}$: Fossil fuel f input coefficient to hydrocarbon production technology $m \in m_h$ per unit of hydrocarbon h

After establishing sufficient fossil fuel availability for all hydrocarbon production, Eq.s 55-63 calculate the total fossil fuel extraction requirements and allocate these flows across polymers, enabling tracking of feedstock use from extraction through final products.

$$F_{f,t} = \sum_h HC_{m,h,t} * \beta 5_{m,f,h}, m \in m_h \quad \text{(Eq.55)}$$

$$F_{f,h,t} = HC_{m,h,t} * \beta 5_{m,f,h}, m \in m_h \quad \text{(Eq.56)}$$

$$F_{f,h,i,t} = HC_{m,h,i,t} * \beta 5_{m,f,h}, m \in m_h \quad \text{(Eq.57)}$$

$$F_{f,h,i,p,t} = HC_{m,h,i,p,t} * \beta 5_{m,f,h}, m \in m_h \quad \text{(Eq.58)}$$

$$F_{f,p,t} = \sum_h \sum_i F_{f,h,i,p,t} \quad \text{(Eq.59)}$$

$$F_{m,f,t} = F_{f,t} * \alpha 5_{m,f,t}, m \in m_f \quad \text{(Eq.60)}$$

$$F_{m,f,h,t} = F_{f,h,t} * \alpha 5_{m,f,t}, m \in m_f \quad \text{(Eq.61)}$$

$$F_{m,f,h,i,t} = F_{f,h,i,t} * \alpha 5_{m,f,t}, m \in m_f \quad \text{(Eq.62)}$$

$$F_{m,f,h,i,p,t} = F_{f,h,i,p,t} * \alpha 5_{m,f,t}, m \in m_f \quad \text{(Eq.63)}$$

where:

$F_{f,t}$: Total demand of fossil fuel f in year t

$F_{f,h,t}$: Demand of fossil fuel f for hydrocarbon h in year t

$F_{f,h,i,t}$: Demand of fossil fuel f for hydrocarbon h to be used in production of monomer i in year t

$F_{f,h,i,p,t}$: Demand of fossil fuel f for hydrocarbon h to be used in production of monomer i and subsequently in polymer p in year t

$HC_{f,p,t}$: Total demand of fossil fuel f for polymer p in year t,

$F_{m,f,t}$: Production of fossil fuel f by fossil fuel extraction/mining technology $m \in m_f$ in year t

$F_{m,f,h,t}$: Production of fossil fuel f by fossil fuel extraction/mining technology $m \in m_f$ for use in production of hydrocarbon h in year t

$F_{m,f,h,i,t}$: Production of fossil fuel f by fossil fuel extraction/mining technology $m \in m_f$ for use in production of hydrocarbon h and subsequently in monomer i in year t

$F_{m,f,h,i,p,t}$: Production of fossil fuel f by fossil fuel extraction/mining technology $m \in m_f$ for use in production of hydrocarbon h and subsequently in monomer i and polymer p in year t
f: Fossil fuel types (crude oil, natural gas, coal)
m_f: Set of fossil fuel extraction/mining technologies

Emission factors for fossil fuel extraction

Eq.s 64-66 calculate GHG emissions from fossil fuel extraction and mining for feedstock use, applying these emission intensities to the fossil fuel production volumes determined in the previous equations.

$$Emis_{f,h,i,p,t} = \sum_{m \in m_f} F_{m,f,h,i,p,t} * \varepsilon_{m,f} \quad \text{(Eq.64)}$$

$$Emis_{f,i,p,t} = \sum_{m \in m_f} F_{m,f,i,p,t} * \varepsilon_{m,f} \quad \text{(Eq.65)}$$

$$Emis_{f,p,t} = \sum_{m \in m_f} F_{m,f,p,t} * \varepsilon_{m,f} \quad \text{(Eq.66)}$$

where:

$Emis_{f,h,i,p,t}$: Total GHG emissions from extraction/mining of fossil fuel f for hydrocarbon h and subsequently for monomer i and polymer p in year t
$Emis_{f,i,p,t}$: Total GHG emissions from extraction/mining of fossil fuel f for monomer i and subsequently for polymer p in year t
$Emis_{f,p,t}$: Total GHG emissions from extraction/mining of fossil fuel f for polymer p in year t
$\varepsilon_{m,f}$: GHG emission intensity of technology $m \in m_f$ used for extraction/mining of fossil fuel f (*e.g., kgCO2e/kg product*),
f: Fossil fuel feedstock type (crude oil, natural gas, coal).

Energy demand

Beyond serving as feedstock, fossil fuels are also extracted to provide process heat throughout the plastic production value chain. Eq. 67 aggregates fuel consumption for process heat across all production stages (excluding electricity, which is treated separately). Eq.s 68-70 convert this energy demand into fossil fuel extraction requirements and calculate associated emissions.

$$E_{e,p,t} = \sum_{m \in m_{pp}} E_{m,p,t} * e_{share_{m,e}} + \sum_{m \in m_p} E_{m,p,t} * e_{share_{m,e}} + \sum_{m \in m_i} E_{m,i\ or\ h',p,t} * e_{share_{m,e}} + \sum_{m \in m_h} E_{m,h,i,p,t} * e_{share_{m,e}} + \sum_{m \in m_c} E_{m,c,i,p,t} * e_{share_{m,e}} \quad \text{(Eq.67)}$$

$$F_{f,p,t} = \sum_{e\ from\ f} E_{e,p,t} / heatvalue(e,f) \quad \text{(Eq.68)}$$

$$F_{f,p,t} = \sum_{m \in m_f} F_{m,f,p,t} \quad \text{(Eq.69)}$$

$$Emis_{f,p,t} = \sum_{m \in m_f} F_{m,f,p,t} * \varepsilon_{m,f} \quad \text{(Eq.70)}$$

where:

$E_{e,p,t}$: Total energy demand for fuel e as process heat for production of plastic product p in year t across the production value chain

$F_{f,p,t}$: Total demand for fossil fuel f extraction converted from energy demand for plastic product p in year t across the production value chain

$Emis_{f,p,t}$: Total GHG emissions from production of fossil fuel f converted from energy demand for plastic product p in year t,

$heatvalue_{e,f}$: heat value e of fossil fuel f *(e.g., MJ/kg)*

$\varepsilon_{m,f}$: GHG emission intensity of technology $m \in m_f$ used for extraction/mining of fossil fuel f *(e.g., kgCO2e/kg product)*

Note: The modeling assumes that global grid emission factors for electricity use already include upstream emissions from fossil fuel extraction for electricity generation. Electricity-related emissions are therefore not double-counted in this fossil fuel extraction stage. For additional details on fossil fuel extraction and mining modeling, refer to the main report.