Petrochemicals Calculator model documentation

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Table of contents

1 Introduction

The goal of the Petrochemicals Calculator model is to give a consistent account of demand, recycling, production of key chemicals, and feedstocks. It ensures mass balance and clearly represents physical process characteristics (e.g. stoichiometry of reactions and yields, and utility requirements), as a basis for calculating lifecycle GHG emissions. The model aims to be able to represent today's state of the system, and as wide a range of future configurations as are feasible. The system scope covers detailed demand-driven modelling of plastics and nitrogen fertilisers, with other chemical demand accounted for in a simplified way, so that total production of primary chemicals is correctly captured. The scope of emissions modelled covers upstream production of feedstocks, indirect emissions from electricity use, emissions from utility combustion and reactions during production of chemicals, nitrogen fertiliser use-phase emissions, and emissions from end-of-life management of waste polymers.

To do this, the model has three main elements, which are described in the following sections of this documentation:

1. The *structure* of the system and the bottom-up processes and objects that it consists of Chapter 2;
2. The *model logic*, which determines how demand and supply are balanced, and which process routes are selected when multiple options are available Chapter 3; and
3. The *levers* that determine how the model configurations evolve over time, aiming to represent scenarios spanning "business as usual" to "maximum possible" (remaining sections of the documentation).

2 System definitions

The “system definitions” include definitions for the process and object types used in the model, and the quantitative recipes for process inputs and outputs.

See the accompanying *System Definitions* document for full documentation.

3 Model logic

The model first calculates the operation of each process based on balancing mass flows (Section 3.1). From this, utility requirements (Section 3.2) are calculated, and hence emissions and other metrics are calculated (Section 3.3).

3.1 Mass-flow process model

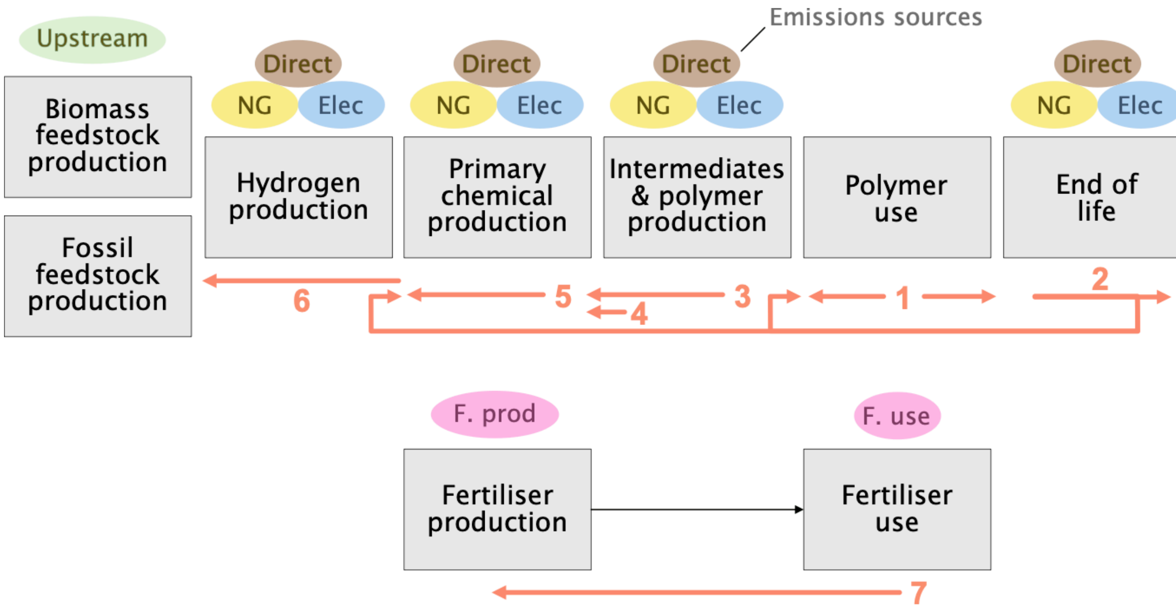


Figure 3.1: Model structure and logic steps

The processes described in Chapter 2 need to be deployed in suitable combinations to meet demand within the available supply and/or capacity constraints. Generally, there are multiple ways that this could plausibly happen, especially when there are multiple technologies available to produce the same chemical. The model "logic" sets out the mass-flow solutions corresponding to particular choices of model parameters (such as capacities or feedstock shares). This builds up the final pattern of process operation and mass flows step by step, as illustrated in Figure 3.1 and described below:

1. Determine demand and end-of-life flows of polymers from the stock model (see Chapter 7).
2. Allocate end-of-life polymers to mechanical recycling or chemical recycling based on the recycling rate parameters, with the residual allocated to final treatment options (see Chapter 8, Chapter 9).
3. Determine required primary chemicals to satisfy the remaining demand for polymers that is not already covered by mechanical recycling. Mechanical recycling is assumed to perfectly substitute virgin polymer production.
4. Add in additional demand for primary chemicals to non-polymer applications (see Chapter 10).
5. Produce primary chemicals in turn using preferred routes first, until their capacity has been exhausted. First, ethylene demand is satisfied:

    - Ethylene is produced from biomass via ethyl alcohol, where capacity is available (see Chapter 13).
    - Ethylene is produced from methyl alcohol (methanol), where MTO capacity is available (see Chapter 11).
    - Any residual demand for ethylene is produced from steam cracking of fossil naphtha and ethane (see Chapter 16).

    These processes produce benzene, toluene, and xylenes (BTX) as by-products; if further demand for BTX remains, then it is satisfied as follows:

    - Demand for xylenes is satisfied from methyl alcohol, where MTA capacity is available (see Chapter 12).
    - Excess toluene production is converted to xylenes by disproportionation.
    - Remaining demand for BTX is produced via catalytic reforming of naphtha, with dealkylation and disproportionation used to balance the mix of BTX as far as possible.

    Finally, on-purpose production of propylene and butadiene is deployed if insufficient supply has already been produced as by-products above:

    - Propylene is produced from methanol (MTP) is additional capacity is still available (see Chapter 11), falling back on dehydrogenation of propane.
    - Butadiene is produced from distillation of excess butylenes supply as co-product of previous processes, if available, falling back on dehydrogenation of butane.

6. Now upstream production is determined, starting with supply of methyl alcohol:

    - Methyl alcohol is produced from green hydrogen when capacity is available (see Chapter 17).
    - Any remaining demand for methyl alcohol is produced from syngas, as below.

Syngas is produced from biomass or fossil feedstocks:

- Syngas is produced from gasification of crop residues where capacity is available (see Chapter 14).
- Any remaining demand for syngas is produced from natural gas and coal.

Remaining demand for hydrogen is produced via green (Chapter 17), blue (Chapter 17), and grey routes in order of preference, up to capacity limits.

Fossil paraffins are sourced from oil refining.

7. Separately, fertiliser use is determined according to the scenarios of Gao and Cabrera Serrenho (2023) (see Chapter 4, Chapter 5, Chapter 6).

Overall, this model logic ensures that any setting of the demand and production capacity parameters results in a pattern of process deployment that is mass balanced and broadly technically plausible, considering the mix of process co-products and routes, even when demand patterns change dramatically and assumptions about allocation factors of chemicals to applications are no longer valid.

3.2 Utility requirements

Utility requirements (natural gas and electricity) are calculated for each process by multiplying the process operation, calculated from the mass flow logic above, with utility requirement parameters (see Chapter 22, Chapter 23).

3.3 Emissions calculation

Emissions from electricity use are based on the parameter `EF_Utility_Electricity` (see Chapter 24), with one exception: electricity used for green hydrogen production is assumed to be always supplied by low-carbon electricity at an emissions factor of 7 gCO_{2e}/kWh (Meys et al. 2021).

Emissions from natural gas use are based on the parameter `EF_Utility_NaturalGas` (see Chapter 25), reduced by a combustion emissions abatement factor (see Chapter 21).

Emissions from process reactions are based on emissions factors for CO_2, CH_4 and N_2O (see Chapter 26, Chapter 28), converted to GWP using IPCC AR5 factors of 1, 28 and 265 respectively. Emissions are reduced by a direct process emissions abatement factor (see Chapter 20), with two exceptions: end-of-life incineration emissions abatement is controlled by a separate lever (Chapter 19), and emissions from end-of-life 'mismanagement' are never abated.

The total quantity of emissions abatement capacity that has been used is accumulated and reported as an additional model output.

Upstream emissions associated with feedstock production are calculated using emissions factors (see Chapter 27).

Finally, processes are grouped according to Table 3.1 for reporting emissions totals.

Table 3.1: Process groups for emissions reporting.

Group	Process
biomass	CornStoverGasificationToSyngas
biomass	EthylAlcoholSynthesisFromCornStover
biomass	EthylAlcoholSynthesisFromMaize
biomass	EthylAlcoholSynthesisFromRiceStraw
biomass	EthylAlcoholSynthesisFromSugarcane
biomass	EthylAlcoholSynthesisFromSugarcaneBagasse
biomass	EthylAlcoholSynthesisFromWheatStraw
biomass	RiceStrawGasificationToSyngas
biomass	SugarCaneBagasseGasificationToSyngas
biomass	WheatStrawGasificationToSyngas
downstream	PolymerisationOfFibrePPA
downstream	PolymerisationOfHDPE
downstream	PolymerisationOfLDPE
downstream	PolymerisationOfLLDPE
downstream	PolymerisationOfOtherPolymers
downstream	PolymerisationOfPET
downstream	PolymerisationOfPP
downstream	PolymerisationOfPUR
downstream	PolymerisationOfPVC
downstream	PolymerisationOfPolystyrene
downstream	PolymerisationOfStyreneButadiene
end_of_life	ChemicalRecyclingOfMixedPolymersAtEOL
end_of_life	Incineration
end_of_life	Landfilling
end_of_life	MechanicalRecyclingOfFibrePPAAtEOL
end_of_life	MechanicalRecyclingOfHDPEPolyethyleneAtEOL
end_of_life	MechanicalRecyclingOfLDPEPolyethyleneAtEOL
end_of_life	MechanicalRecyclingOfLLDPEAtEOL
end_of_life	MechanicalRecyclingOfPETPolyethyleneTerephthalatePolyestersAtEOL
end_of_life	MechanicalRecyclingOfPPPolypropyleneAtEOL
end_of_life	MechanicalRecyclingOfPSPolystyreneAtEOL
end_of_life	MechanicalRecyclingOfPVCPolyvinylChlorideAtEOL

Table 3.1: Process groups for emissions reporting.

Group	Process
end_of_life	Mismanagement
green_hydrogen	WaterElectrolysisForHydrogen
organic_synthesis	AceticAcidSynthesis
organic_synthesis	AcrylonitrileSynthesis
organic_synthesis	AdipicAcidSynthesis
organic_synthesis	CyclohexaneSynthesis
organic_synthesis	EthyleneGlycolSynthesis
organic_synthesis	EthyleneOxideSynthesis
organic_synthesis	HexamethylenediamineSynthesisFromButadiene
organic_synthesis	HydrogenCyanideSynthesis
organic_synthesis	IsophthalicAcidSynthesis
organic_synthesis	OtherOrganicChemicalsSynthesis
organic_synthesis	PolyolsSynthesis
organic_synthesis	PropyleneOxideSynthesis
organic_synthesis	StyreneSynthesis
organic_synthesis	TerephthalicAcidSynthesis
organic_synthesis	TolueneDiisocyanateSynthesis
organic_synthesis	VinylChlorideSynthesis
other_hydrogen	NaturalGasSteamMethaneReformingToHydrogen
other_hydrogen	NaturalGasSteamMethaneReformingWithCCSToHydrogen
primary_production	CarbonDioxideHydrogenationToMethylAlcohol
primary_production	CatalyticReformingOfNaphthaForToluene
primary_production	CatalyticReformingOfNaphthaForXylenes
primary_production	CoalGasificationToSyngas
primary_production	DealkylationOfTolueneForBenzene
primary_production	DehydrationOfEthylAlcohol
primary_production	DehydrogenationOfButaneForButadiene
primary_production	DehydrogenationOfPropane
primary_production	DisproportionationOfTolueneForXylenes
primary_production	DistillationOfButylenesForButadiene
primary_production	DistillationOfPyrolysisGasolineForBTX
primary_production	FischerTropschSynthesisOfOlefinsFromSyngas
primary_production	FluidCatalyticCrackingOfGasOil
primary_production	MethylAlcoholSynthesis
primary_production	MethylAlcoholToAromatics
primary_production	MethylAlcoholToOlefins
primary_production	MethylAlcoholToPropylene
primary_production	NaturalGasSteamMethaneReformingToSyngas
primary_production	SodiumChlorideElectrolysisForChlorine

Table 3.1: Process groups for emissions reporting.

Group	Process
primary_production	SteamCrackingOfEthane
primary_production	SteamCrackingOfNaphtha
primary_production	SyngasToAmmoniaProduction

Emissions from fertiliser production are calculated directly from the production quantity of each fertiliser type (see Chapter 4), and production & use-phase emissions factors (see Chapter 5, Chapter 6).

Part I

Fertilisers

4 fertiliser_demand

Lever ID fertiliser_demand
Description Fertiliser demand changes
Levels

- *Level 1:* BAU
- *Level 2:* Demand reduction
- *Level 3:* Demand reduction and fertiliser substitution

This lever controls the level of demand for fertilisers globally, based on Gao and Cabrera Serrenho (2023).

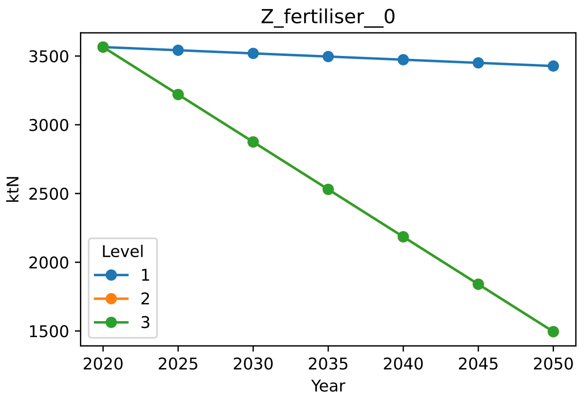
The regional total demand for synthetic nitrogen fertilisers in the BAU scenario in 2050 is extracted from the forecast made by the FAO (2022). The fractions of various nitrogen fertiliser are estimated using the regional fractions in 2019.

The regional total demand for synthetic nitrogen fertilisers in the demand reduction scenario is calculated by the authors, considering optimistic nitrogen use efficiency. More details are be found in Gao and Cabrera Serrenho (2023). Again, the fractions of nitrogen fertilizers are estimated using the regional fractions in 2019.

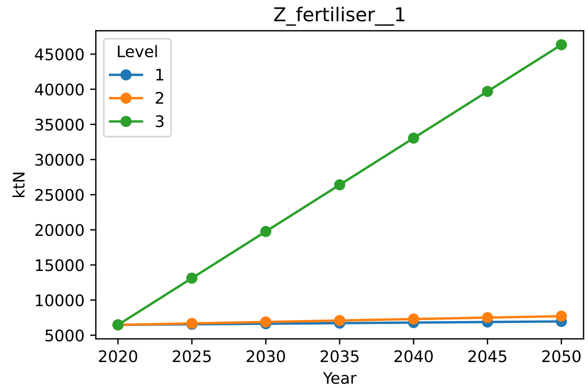
The regional total demand for synthetic nitrogen fertilizers in the demand reduction and fertiliser substitution scenario is the same as the demand reduction scenario, while the fractions are different. To gradually get rid of high-emitting nitrogen fertilisers, the fractions of urea, urea ammonium nitrate (UAN) and other nitrogen fertilisers (represented by ammonium bicarbonate in the study), are linearly interpolated from current values in 2020 to zero in 2050. Their contributions are made up by ammonium nitrate (AN).

4.1 Parameter data

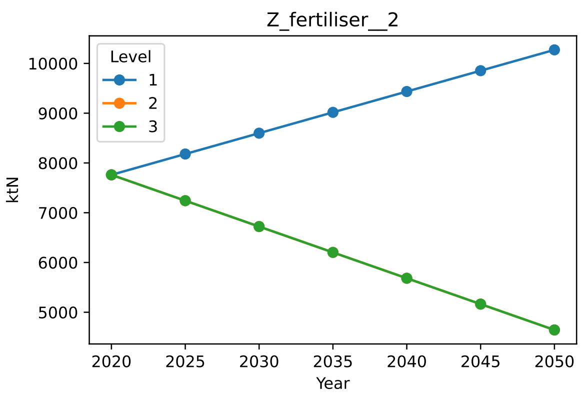
The plots below show the value over time of each parameter affected by this lever.



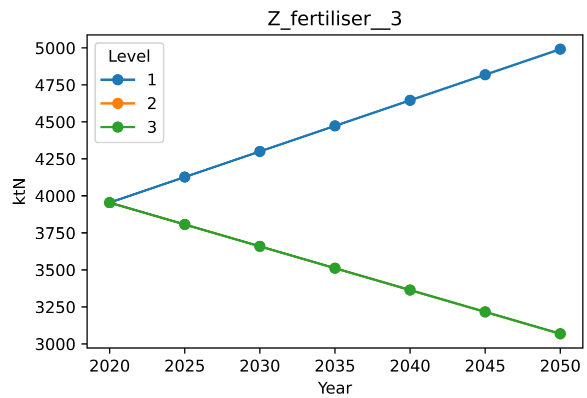
(a) Production of AmmoniaFertiliser



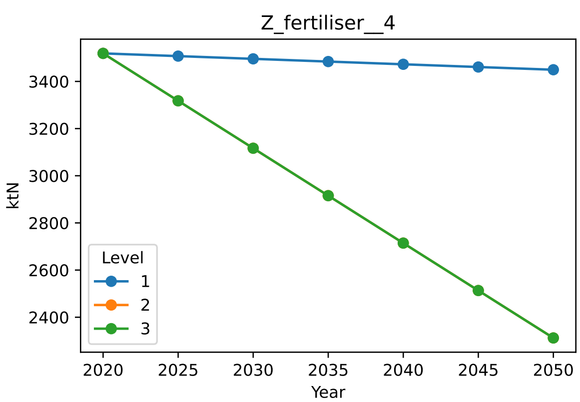
(b) Production of AmmoniumSulphate



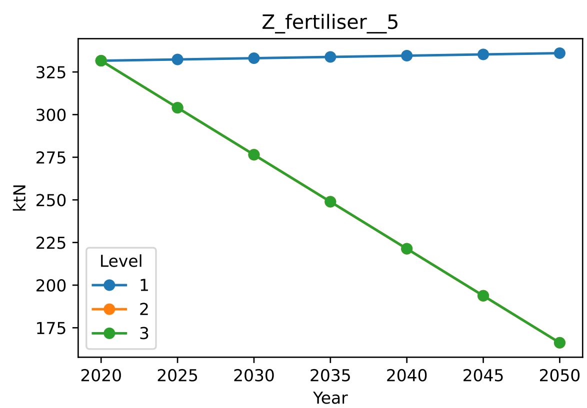
(c) Production of AmmoniumNitrate



(d) Production of CalciumAmmoniumNitrate

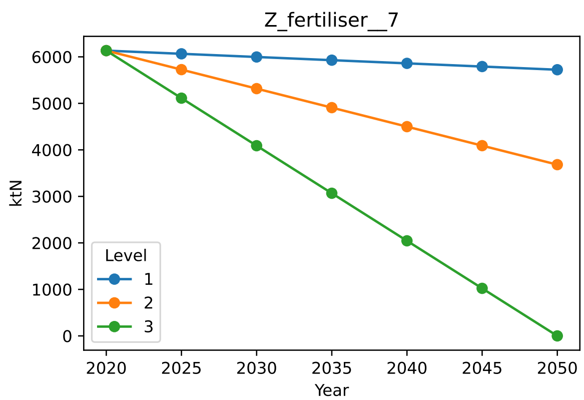


(e) Production of AmmoniumPhosphate

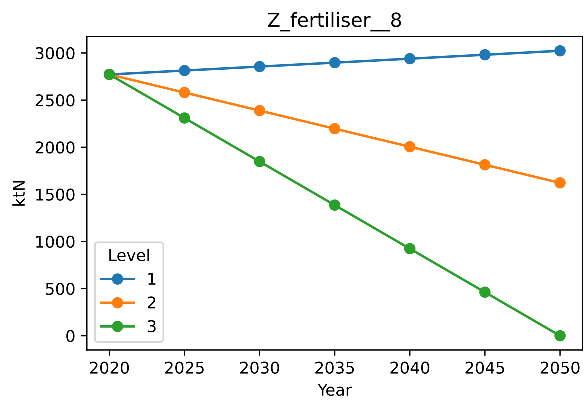


(f) Production of NKCompound

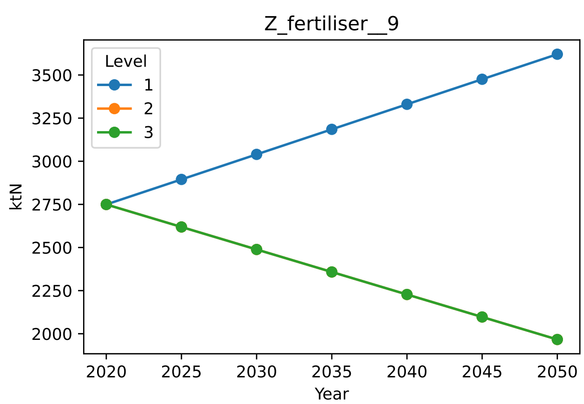
Figure 4.1: `fertiliser_demand` parameter data (part 1)



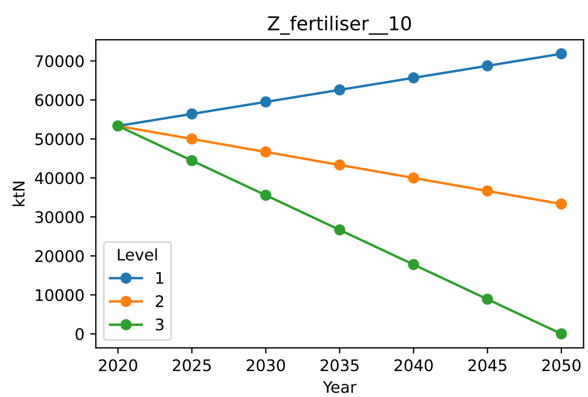
(a) Production of NPKCompound



(b) Production of UreaAmmoniumNitrate



(c) Production of OtherFertiliserN



(d) Production of OtherFertiliserNP

Figure 4.2: `fertiliser_demand` parameter data (part 2)

5 fertiliser_production

Lever ID fertiliser_production
Description Fertiliser production changes
Levels

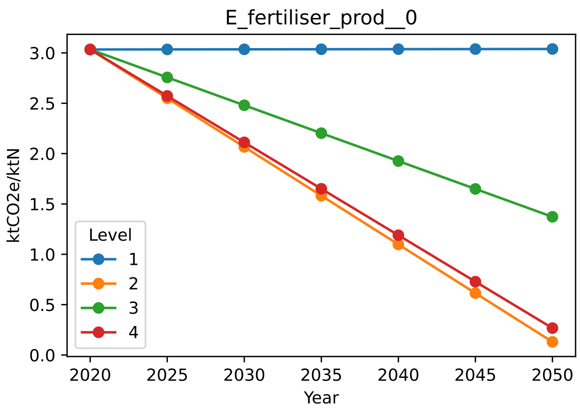
- *Level 1:* BAU
- *Level 2:* Water electrolysis
- *Level 3:* Electrical heating
- *Level 4:* CCS

This lever controls the emissions factor for fertilisers production, based on Gao and Cabrera Serrenho (2023).

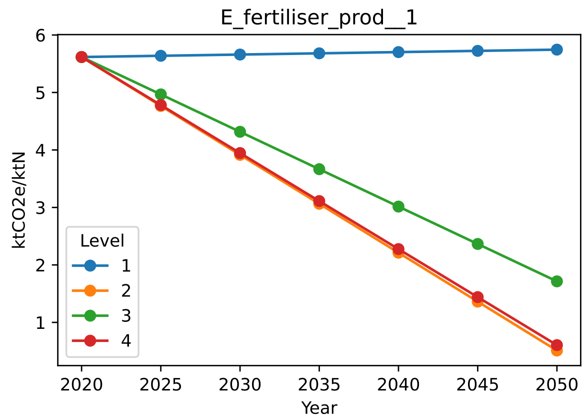
The production emission factors of various nitrogen fertilisers are constant in the BAU scenario. The production emission factors of each nitrogen fertiliser in water electrolysis, electrical heating and CCS scenarios in 2050 are estimated in our previous study (Gao and Cabrera Serrenho 2023). Note that the electrolysis scenario also includes electrical heating, while the CCS scenario is independent of other scenarios. The emission factors are linearly interpolated from 2020 to 2050.

5.1 Parameter data

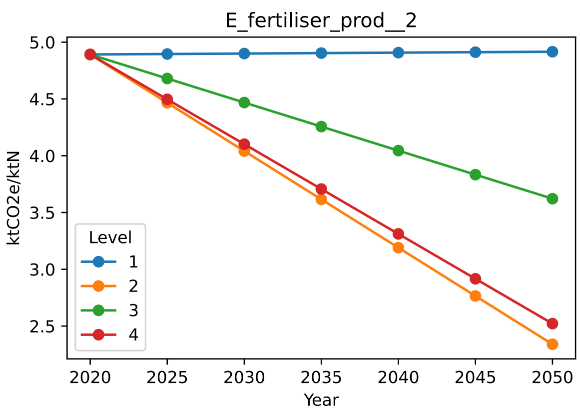
The plots below show the value over time of each parameter affected by this lever.



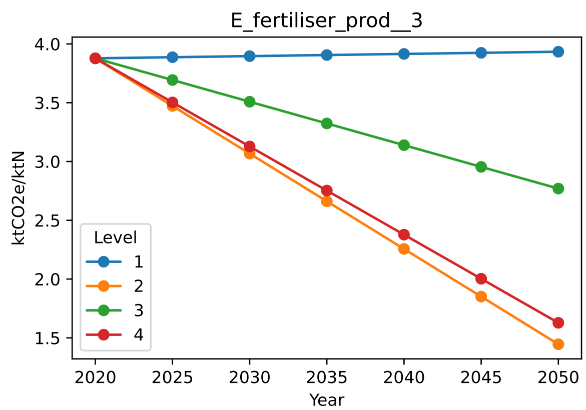
(a) Production of AmmoniaFertiliser



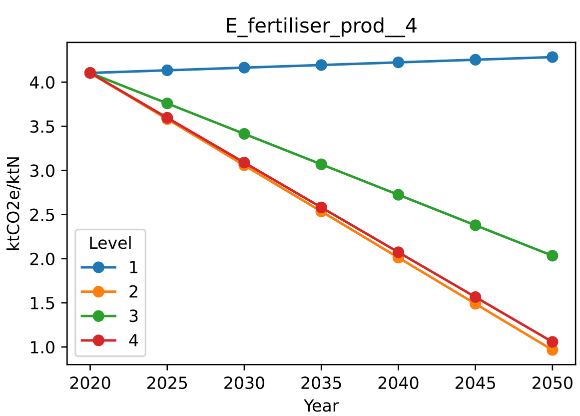
(b) Production of AmmoniumSulphate



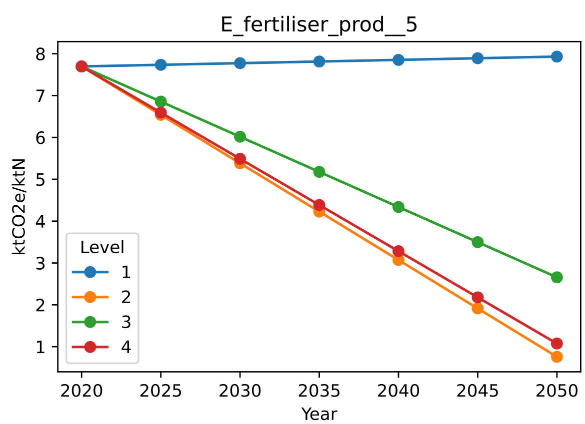
(c) Production of AmmoniumNitrate



(d) Production of CalciumAmmoniumNitrate

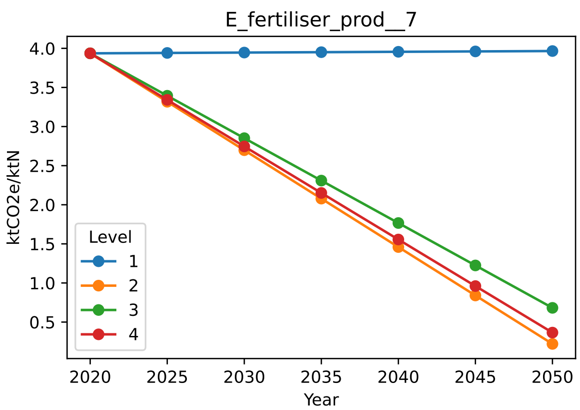


(e) Production of AmmoniumPhosphate

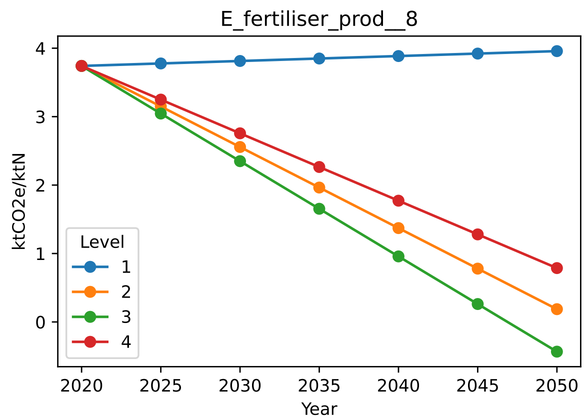


(f) Production of NKCompound

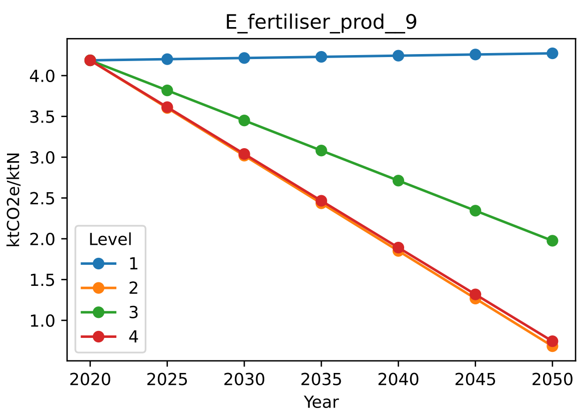
Figure 5.1: `fertiliser_production` parameter data (part 1)



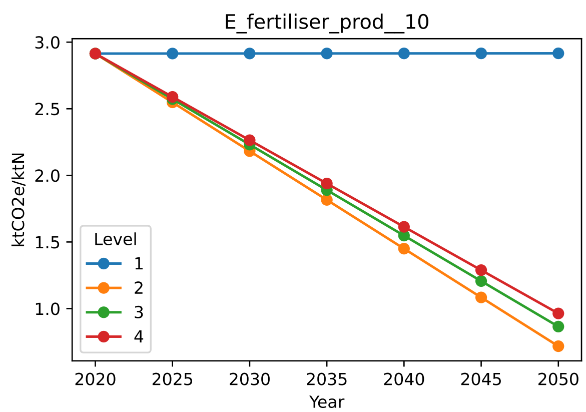
(a) Production of NPKCompound



(b) Production of UreaAmmoniumNitrate



(c) Production of OtherFertiliserN



(d) Production of OtherFertiliserNP

Figure 5.2: `fertiliser_production` parameter data (part 2)

6 fertiliser_use_phase

Lever ID fertiliser_use_phase
Description Fertiliser use-phase changes
Levels

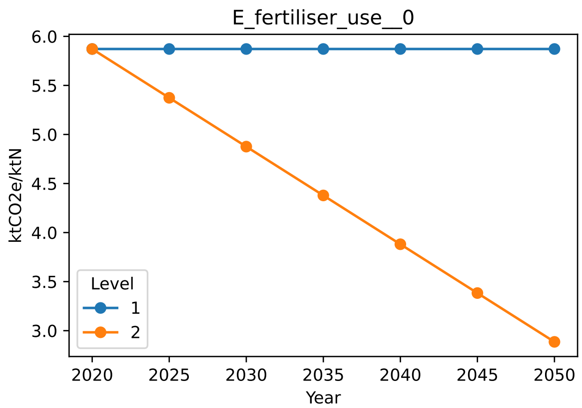
- *Level 1:* BAU
- *Level 2:* Nitrification inhibitor

This lever controls the emissions factor for fertilisers use, based on Gao and Cabrera Serrenho (2023).

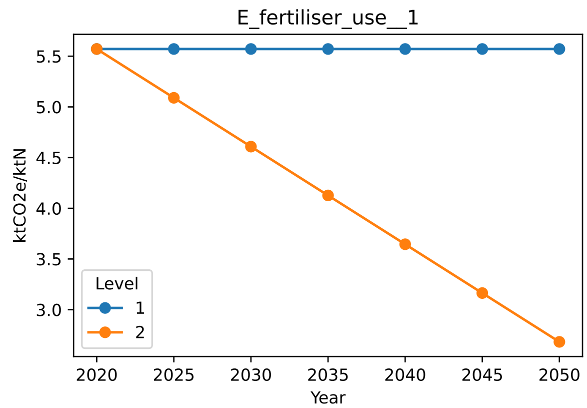
The use-phase emission factors of various nitrogen fertilisers are constant in the BAU scenario. In the nitrification inhibitor scenario, the use-phase emission factors in 2050 are calculated in our previous study (Gao and Cabrera Serrenho 2023). The use-phase emission factors are linearly interpolated from 2020 to 2050.

6.1 Parameter data

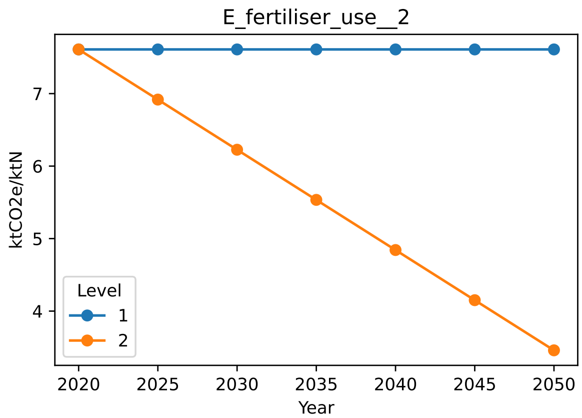
The plots below show the value over time of each parameter affected by this lever.



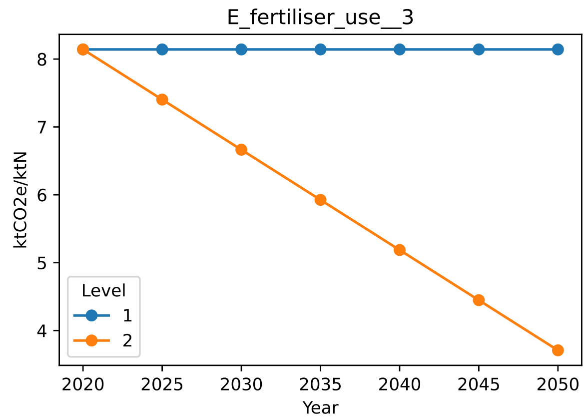
(a) Use of AmmoniaFertiliser



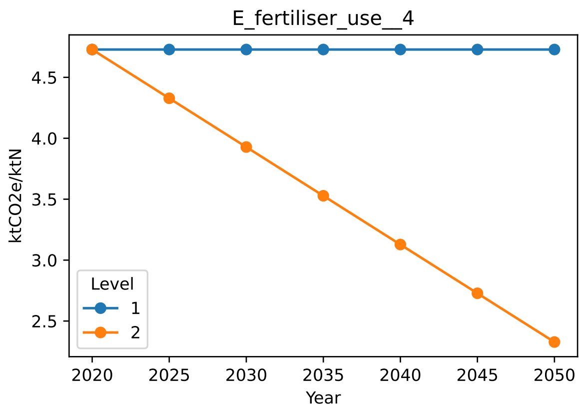
(b) Use of AmmoniumSulphate



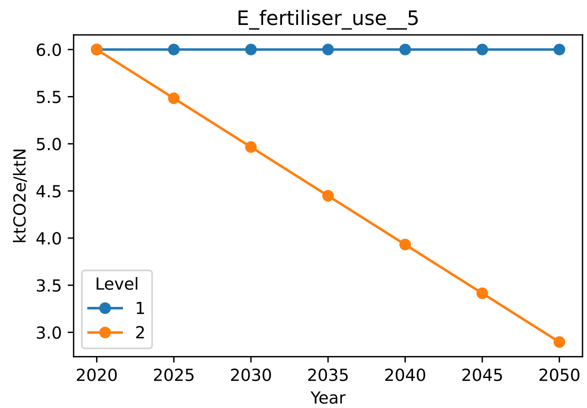
(c) Use of AmmoniumNitrate



(d) Use of CalciumAmmoniumNitrate

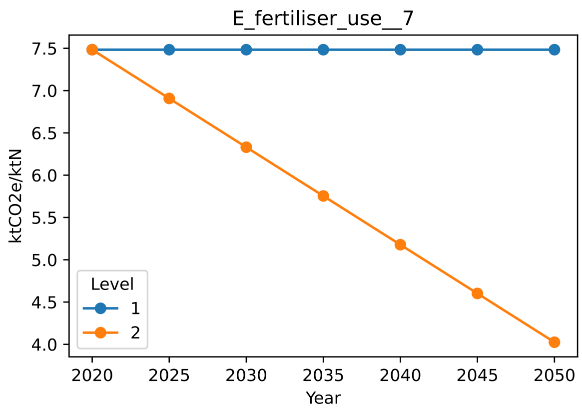


(e) Use of AmmoniumPhosphate

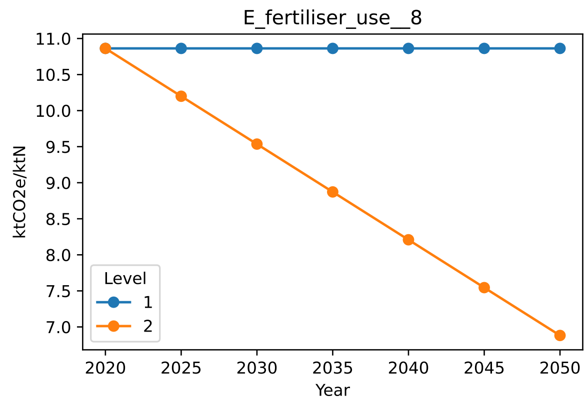


(f) Use of NKCompound

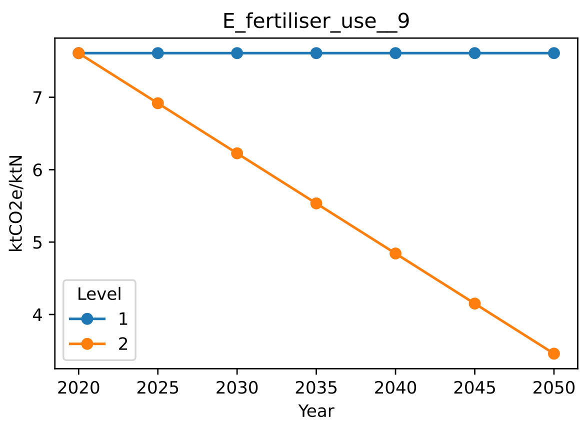
Figure 6.1: `fertiliser_use_phase` parameter data (part 1)



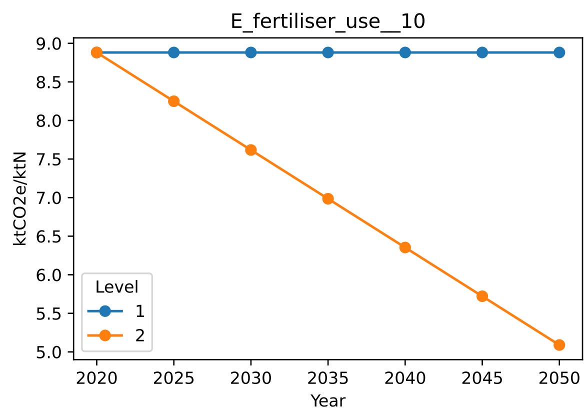
(a) Use of NPKCompound



(b) Use of UreaAmmoniumNitrate



(c) Use of OtherFertiliserN



(d) Use of OtherFertiliserNP

Figure 6.2: `fertiliser_use_phase` parameter data (part 2)

Part II

Demand model levers

7 product_demand

Lever ID product_demand
Description Reduce the quantity of polymer-containing goods required to drive reduced demand for new polymers (and also reduced end-of-life waste)
Levels

- *Level 1:* BAU
- *Level 2:* Stock per capita to 50% of the current North American level
- *Level 3:* Stock per capita to 30% of the current North American level
- *Level 4:* Stock per capita to 10% of the current North American level

This lever describes demand for polymers and end-of-life flows, based on Gao and Cabrera Serrenho (n.d.) stock modelling.

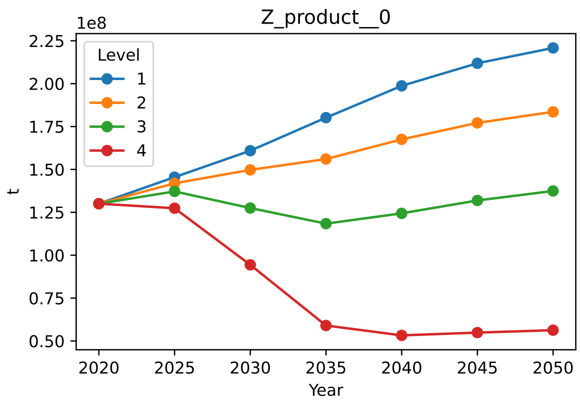
This uses a Dynamic Material Flow Analysis approach based on the assumption that, for durable goods, the per-capita stock of material in use is the more fundamental driver of material demand and waste flows. In the BAU scenario, the historical regional per-capita stock in each sector is correlated with regional GDP per-capita, then forecast to increase as GDP per capita increases per the second Shared Socioeconomic Pathway (Crespo Cuaresma 2017). Coupled with the forecasted population growth by the United Nations (UN 2022), the regional sectoral demand is calculated by adding the yearly change of stock and waste generation.

The percentage demand reduction levels represent a range of conceivable levels of demand reduction, which might be achieved through different specific strategies. The levels refer to the in-use per-capita stock being reduced compared to the current North American level (which in turn drives the material demand and waste flows). More details can be found in Gao and Cabrera Serrenho (n.d.).

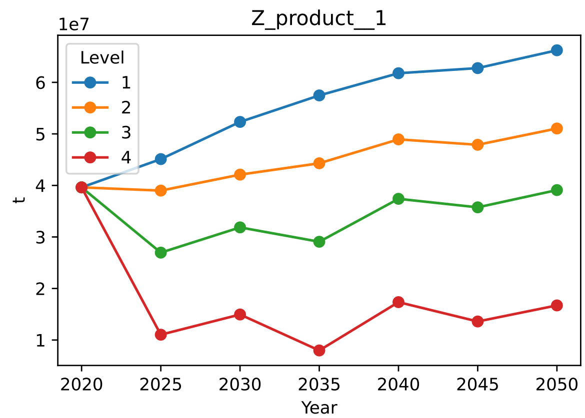
Similarly, for short-lived products such as packaging, the forecasted per-capita input increases as the fitted historical trend and forecasted GDP and population growth in the BAU scenario. In demand reduction scenarios, the regional input flow per capita is assumed to be capped to certain percentages of the current North American level.

7.1 Parameter data

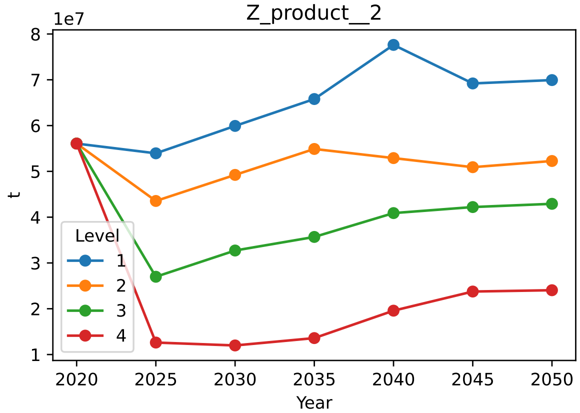
The plots below show the value over time of each parameter affected by this lever.



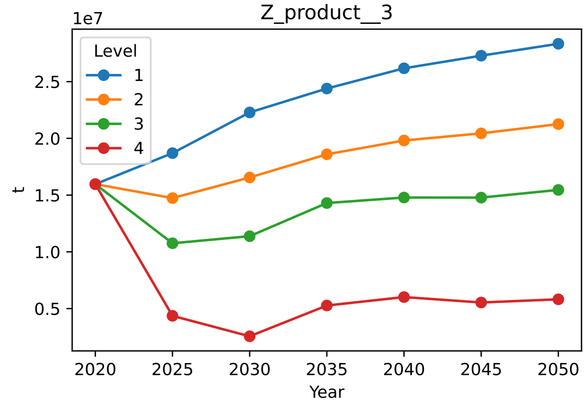
(a) Demand for Packaging



(b) Demand for Transportation

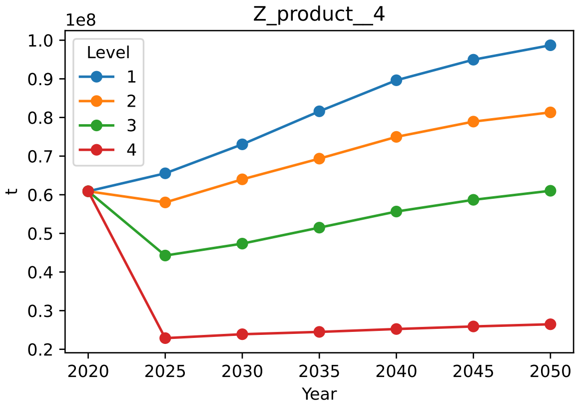


(c) Demand for BuildingsAndConstruction

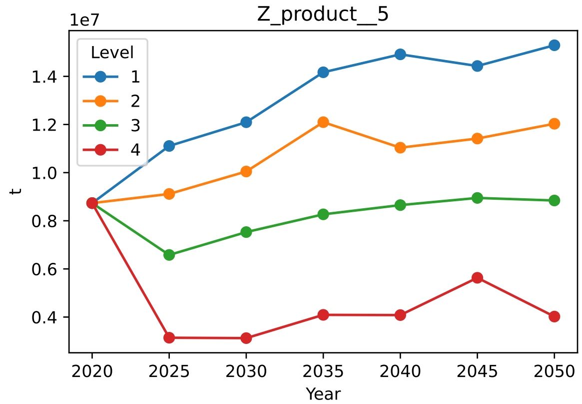


(d) Demand for ElectricalAndElectronic

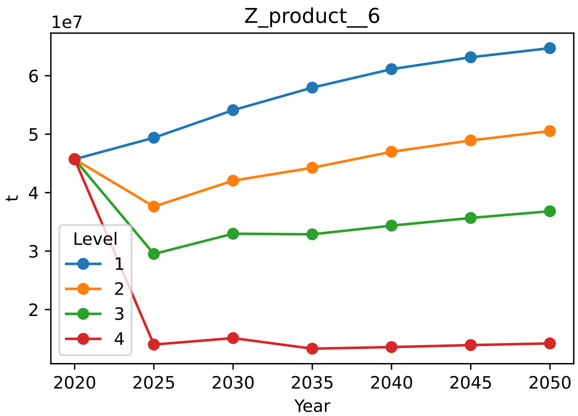
Figure 7.1: `product_demand` parameter data (part 1)



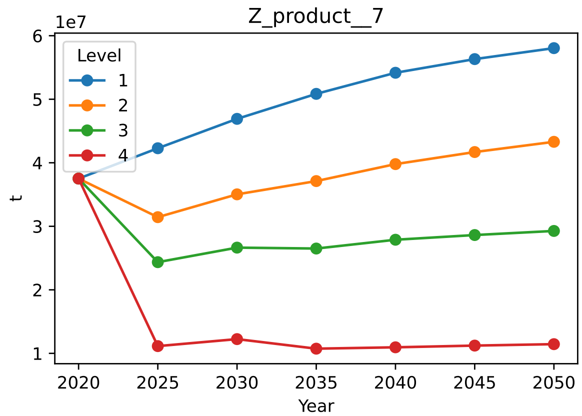
(a) Demand for ConsumerAndInstitutional



(b) Demand for IndustrialMachinery

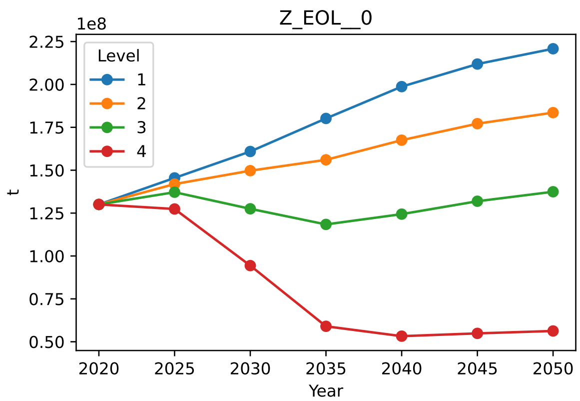


(c) Demand for Textile

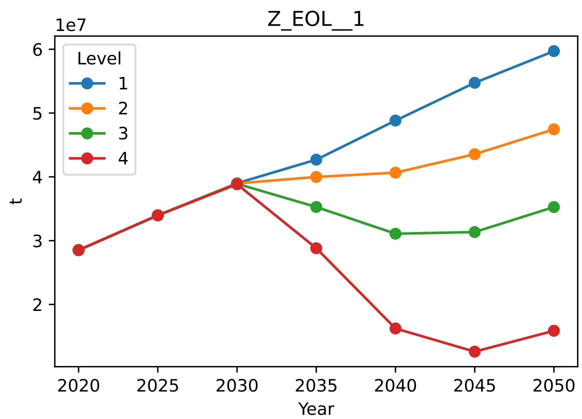


(d) Demand for Other

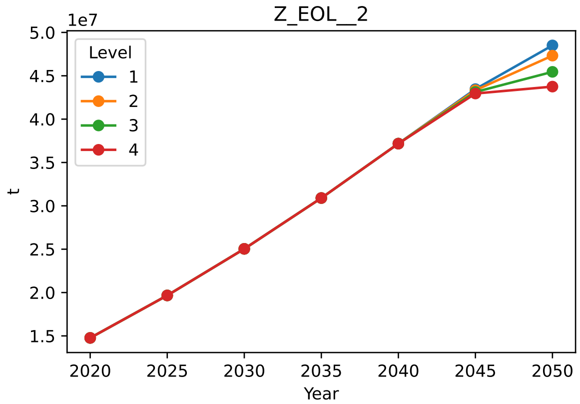
Figure 7.2: `product_demand` parameter data (part 2)



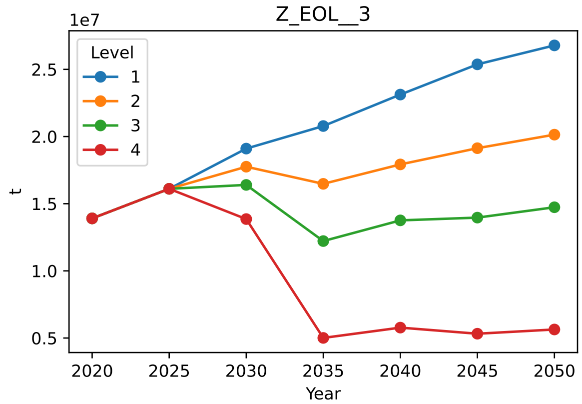
(a) EOL from Packaging



(b) EOL from Transportation

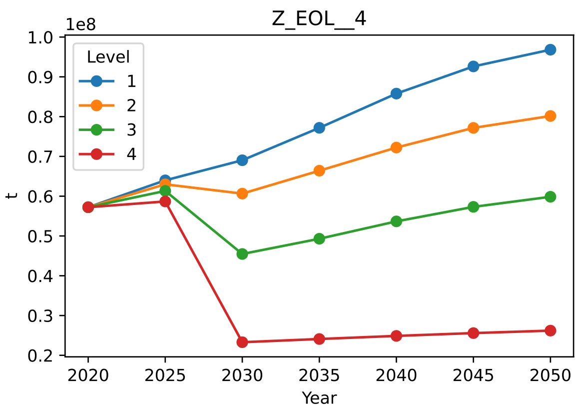


(c) EOL from BuildingsAndConstruction

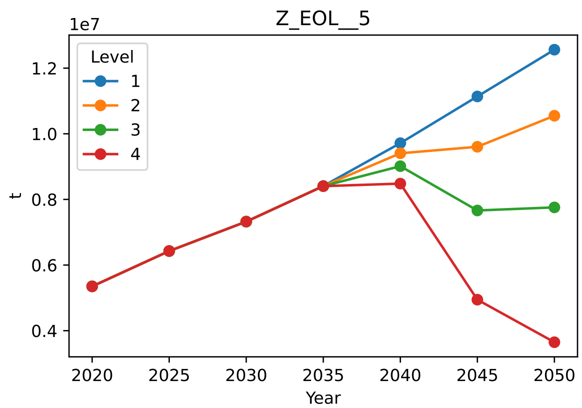


(d) EOL from ElectricalAndElectronic

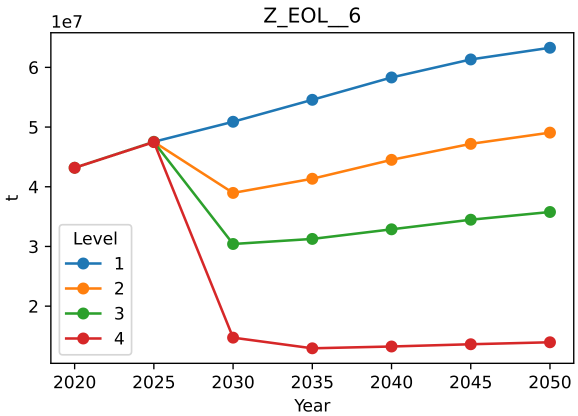
Figure 7.3: `product_demand` parameter data (part 3)



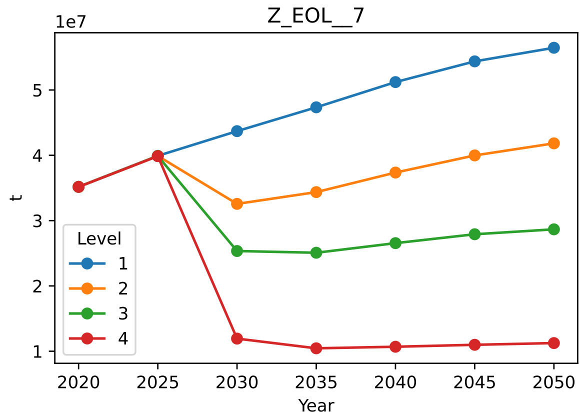
(a) EOL from ConsumerAndInstitutional



(b) EOL from IndustrialMachinery



(c) EOL from Textile



(d) EOL from Other

Figure 7.4: `product_demand` parameter data (part 4)

8 recycling

Lever ID recycling
Description Increase the fraction of end-of-life materials chemically or mechanically recycled
Levels

- *Level 1:* Basline recycling fractions (no chemical recycling)
- *Level 2:* Reference projected recycling fractions
- *Level 3:* Ambitious projected recycling both chemical and mechanical
- *Level 4:* Nearly all waste which cannot be mechanically recycled is chemically recycled

This lever controls recycling rates for each polymer at end-of-life.

Plastics are made of two types of polymers: thermoplastics and thermosets.

- Thermoplastics are made up of single long chains of molecules such as low density polyethylene (LDPE), linear low-density polyethylene (LLDPE), high-density polyethylene (HDPE), polypropylene (PP), polystyrene (PS), polyvinyl chloride (PVC), polyethylene terephthalate (PET), and fibre polyphthalamide (PPA). They can be melted and formed again to original state with little to no loss in properties (Wikipedia 2024a). It makes sense to mechanically recycle them.

- Thermosets involve cross-linking such as polyurethane (PUR) and styrene-butadiene rubber (SBR) or synthetic rubbers. Other polymers were placed under this category for simplicity. Melting them tends to induce curing and can change their properties (Wikipedia 2024b). It does not make sense to mechanical recycle them. They can be downcycled by cutting them up and re-using them, which is not mechanical recycling in this sense as we want them back to their original form and purpose. Hence, chemical recycling that breaks them down to their feedstock and/or monomer makes more sense as these can be used to produce the original polymer back.

Chemical recycling covers both more targeted processes to return polymers to monomers, and broader pyrolysis processes.

8.1 Possible recycling routes

First the possible recycling routes in different scenarios are set for 3 levels of ambition, as summarised in Table 8.1.

Table 8.1: Current, improved and ambitious options for recycling routes by polymer. "M" indicates suitability for mechanical recycling, "C" for chemical recycling.

Polymer type	Current	Practical	Ambitious
LDPE	M / _	M / _	M / C
HDPE	M / _	M / _	M / C
LLDPE	_ / _	M / _	M / C
PET	M / _	M / C	M / C
PP	M / _	M / _	M / C
PVC	_ / _	M / _	M / C
PS	_ / _	M / C	M / C
Fibre PPA	_ / _	_ / C	M / C
PUR	_ / _	_ / C	_ / C
SBR	_ / _	_ / _	_ / C
Other polymers	_ / _	_ / _	_ / C

8.1.1 Current routes

Currently the possibilities for recycling polymers are as follows:

- LDPE, HDPE, and PET are widely recycled (OECD 2018). There is virtually no chemical recycling today (Van Geem 2023): all current recycling is mechanical.
- PP can be mechanically recycled, but only 1% of the world production is recycled. Majority of the discarded PP goes to landfills and oceans (Basham 2019). There is also a misconception that waste PP from health sector cannot be recycled, hence, majority are incinerated without recovering the energy (Healthcare 2019).
- LLDPE can be mechanically and chemically recycled. Because it is often blended with other types of plastics that make its recycling challenging, consequently, its recycling rate is generally low (Arkema 2023). This is also compounded with the dwindling demand for LLDPE and about 60% is for single-use applications, hence, investments on recycling LLDPE needs to be economically justified (Richardson 2018).
- Mechanical recycling is recommended for PVC, but this is not happening now as it is mistaken to have low thermal stability and to generate toxic degradation products, which are misconceptions as it can be widely recycled (Lewandowski and Skórczewska 2022).
- PS can be mechanically and chemically recycled (Maharana, Negi, and Mohanty 2007). Despite being so, PS recycling is not done globally at present, because it is not economically feasible (Marquez et al. 2023) and it is logistically difficult (Waring 2018). Hence, it makes more sense to produce virgin PS than recycle it.

- PUR recycling is not predominantly done, despite the effort from manufacturers and legislators. Most PUR wastes end up in landfills (Kemona and Piotrowska 2020).
- With tire industry representing 65% of the global rubber production, most rubber wastes go to landfills (Fazli and Rodrigue 2020).
- PPA is generally mixed with other plastics, hence, there is limited recycling, with most going to incineration and land filling (Hirschberg and Rodrigue 2023).

8.1.2 Future routes

Expectations for future improvements for each polymer are:

- Following from the current practice: LDPE, HDPE, and PET will continue to be mechanically recycled (OECD 2018).
- LLDPE, PP and PVC can be recycled more, via mechanical recycling (OECD 2018; Lewandowski and Skórczewska 2022).
- PS and PET can be both mechanically and chemically recycled (Maharana, Negi, and Mohanty 2007; Gao and Cabrera Serrenho n.d.).
- Mechanical recycling degrades the polymer properties of PUR (Rossignolo, Malucelli, and Lorenzetti 2024) and PPA (Hirschberg and Rodrigue 2023), so chemical recycling is most appropriate.

This forms the "practical limit" level.

Beyond this, all the rest of the polymers can be chemically recycled provided the technologies became technically, economically, and environmentally feasible. This forms the "ambitious" level.

8.2 Quantifying recycling rates

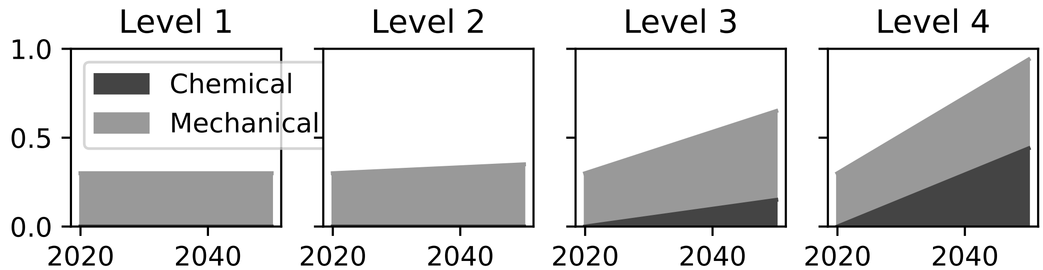
The baseline overall global recycling rate is 9% according to OECD (2022). This is distributed across the relevant polymers for each level Table 8.1 based on the mass flow quantities of each polymer in the baseline model. The recycling rate for PP is 1% (Basham 2019), and equal recycling rates for HDPE, LDPE and PET of 30% was assumed to give an overall mass-weighted recycling rate of 9%.

The reference business-as-usual projection in recycling rate growth from OECD (2022) reaches 16% by 2050. We assume growth in mechanical recycling rates on the polymers already recycled to 15% and 35% respectively. Additional growth in recycling is distributed across the other recycling routes added in this level of Table 8.1 at 15% for LLDPE and 5% for others.

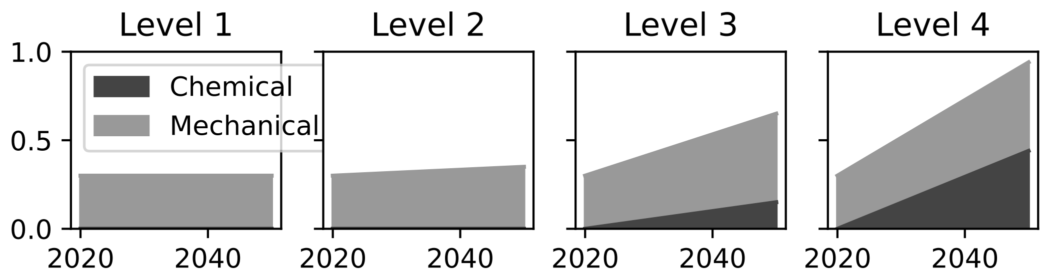
The more ambitious scenario from OECD (2022) reaches 47% overall recycling rate by 2050. This increase is achieved by increasing recycling rates to 50% for all polymers which can be mechanically recycled in Table 8.1, together with 15% chemical recycling of all polymers.

8.3 Parameter data

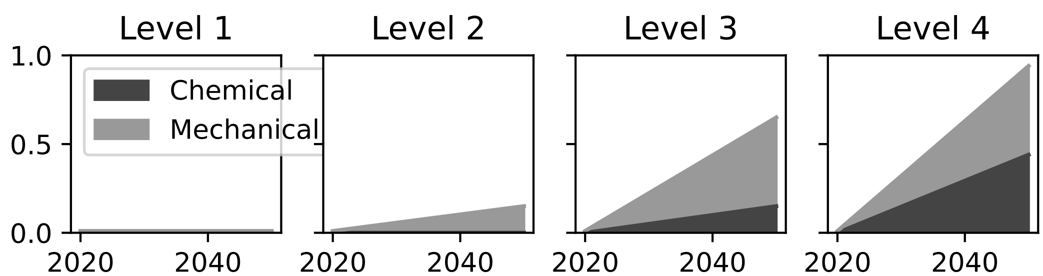
The plots below show the change in recycling rates over time for each polymer affected by this lever.



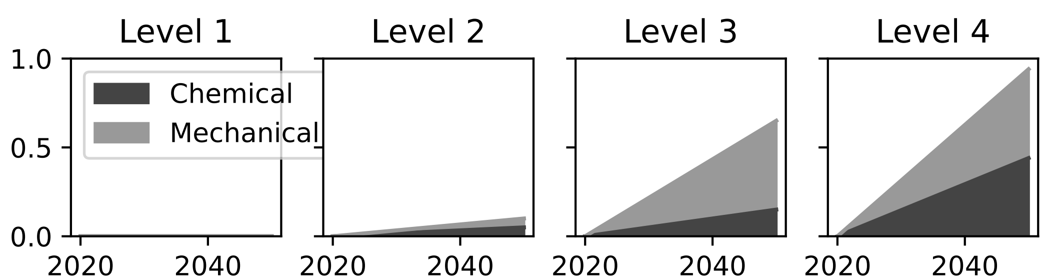
(a) LDPEPolyethylene



(b) HDPEPolyethylene

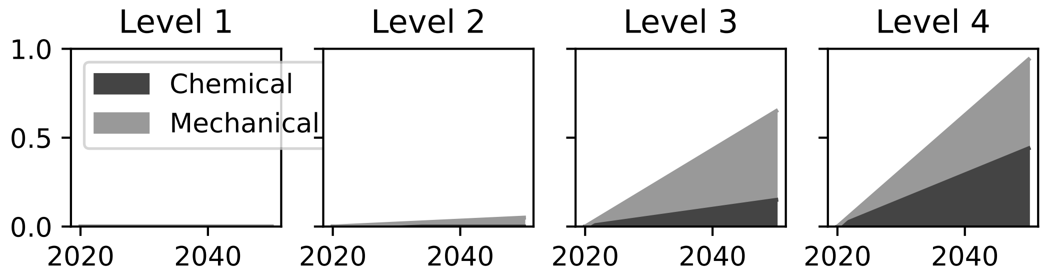


(c) PPPolypropylene

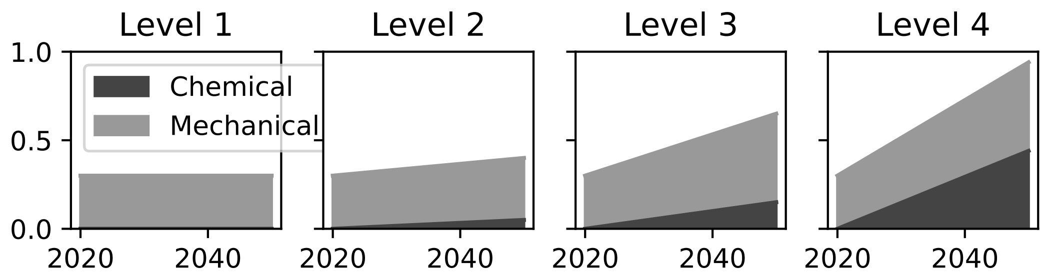


(d) PSPolystyrene

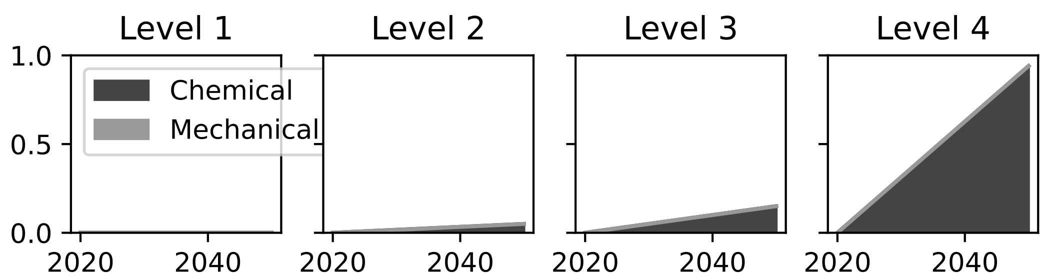
Figure 8.1: `recycling` parameter data (part 1)



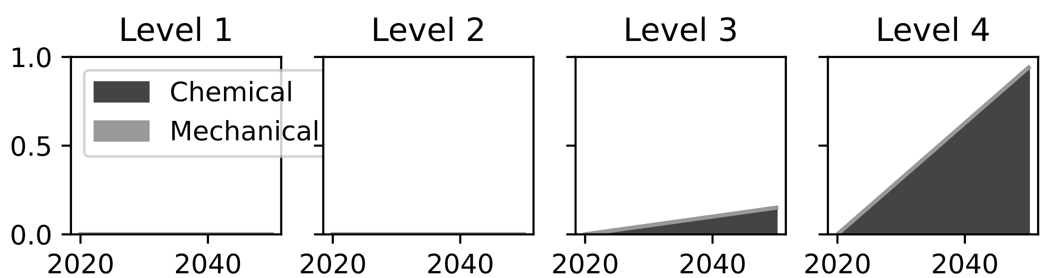
(a) PVCPolyvinylChloride



(b) PETPolyethyleneTerephthalatePolyesters

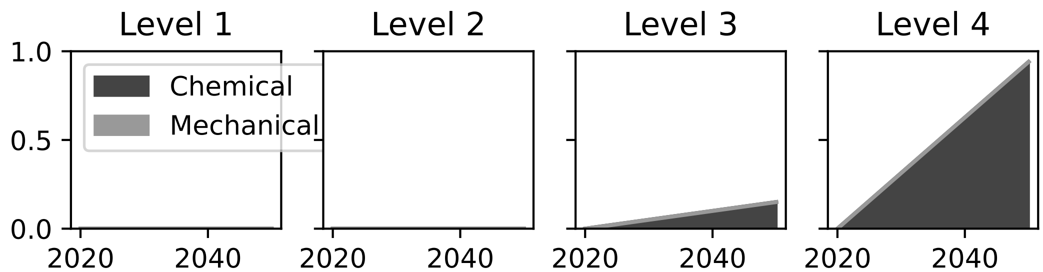


(c) Polyurethane

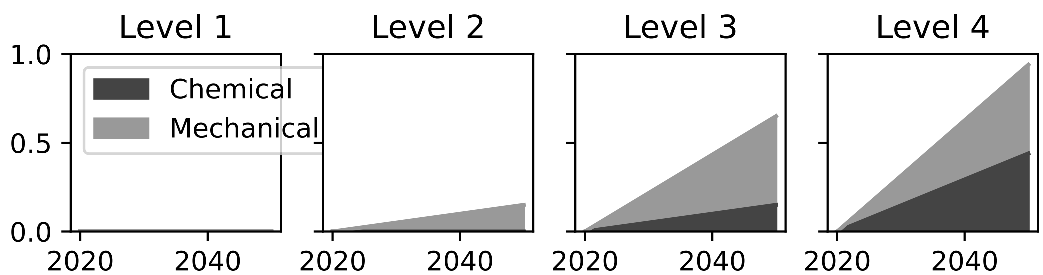


(d) SyntheticRubbers

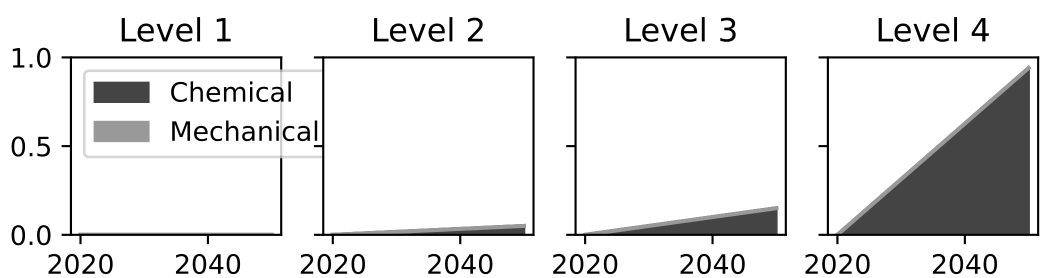
Figure 8.2: `recycling` parameter data (part 2)



(a) OtherPolymers



(b) LLDPE



(c) FibrePPA

Figure 8.3: `recycling` parameter data (part 3)

9 final_treatment

Lever ID final_treatment
Description Divert the end-of-life materials which are NOT recycled to landfill or incineration
Levels

- *Level 1:* Current shares of final treatment options
- *Level 2:* Reference projected fraction of final treatment option
- *Level 3:* High incineration scenario
- *Level 4:* High landfilling scenario

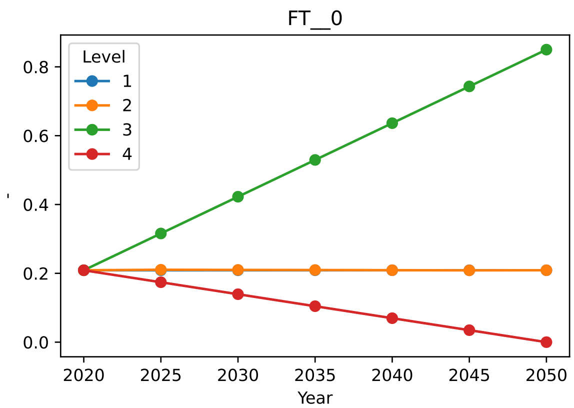
This lever controls how much non-recycled end-of-life material is sent to different destinations.

The current data and reference projection are from OECD (2022).

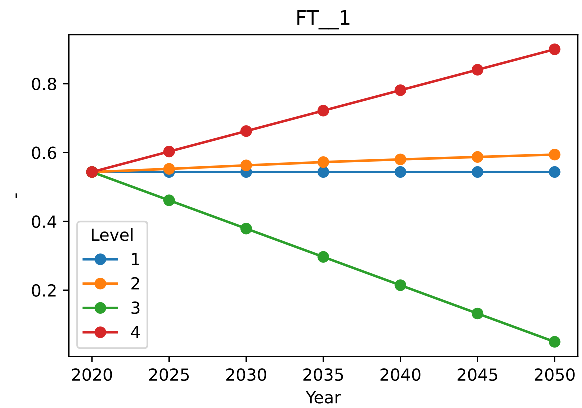
To consider different possible end-of-life options which affect GHG emissions, additional lever levels are added with very high incineration and landfilling shares respectively. A residual 10% share for mismanagement is assumed to persist.

9.1 Parameter data

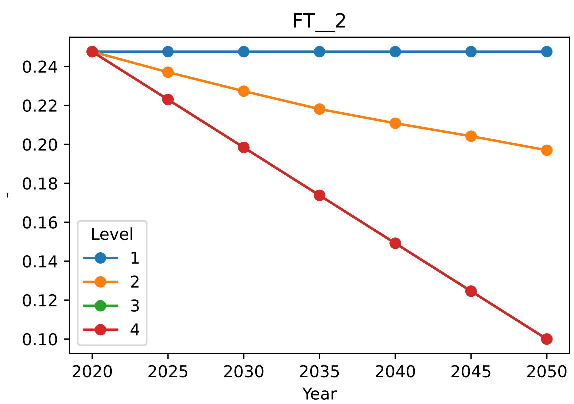
Figure 9.1 shows the value over time of each parameter affected by this lever.



(a) Incineration



(b) Landfilling



(c) Mismanagement

Figure 9.1: `final_treatment` parameter data

10 extra_demand

Lever ID extra_demand

Description Reduce other demands of benzene, toluene, xylenes, and methyl alcohol, not related to polymer production.

Levels

- *Level 1:* Reference projected extra demand
- *Level 2:* Demand reduced to 50% of the current
- *Level 3:* Demand reduced to 30% of the current
- *Level 4:* Demand reduced to 10% of the current

This lever controls reductions in the additional demand for primary chemicals, which is not driven by the main model's demand for polymers, nor the demand of primary chemicals for fertilisers covered by the model of Gao and Cabrera Serrenho (2023).

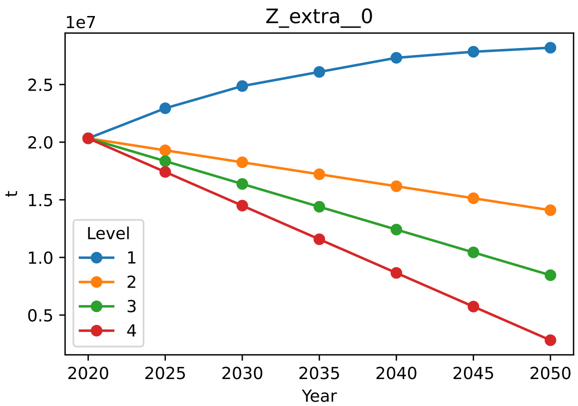
The baseline level of extra demand has been calibrated based on total global demand for BTX (ICIS 2021) and methyl alcohol (Methanol Institute 2023).

The reference projection is based on projected growth in demand for BTX (ICIS 2021), minus the baseline demand in the model of these chemicals for polymers, assuming that the share of this demand which is for non-polymer applications remains constant over time. Methyl alcohol is similar based on projections from Methanol Institute (2023).

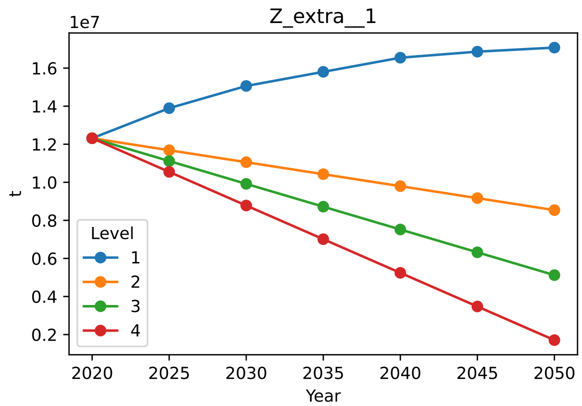
The demand-reduction scenarios then scale down from this projected demand proportionally, to illustrate how different supply-side scenarios are affected by changes in demand levels.

10.1 Parameter data

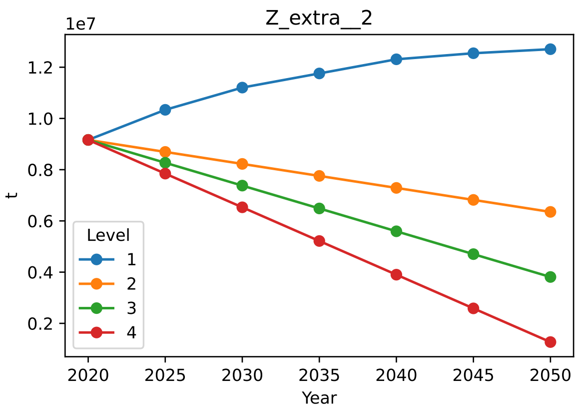
Figure 10.1 shows the value over time of each parameter affected by this lever.



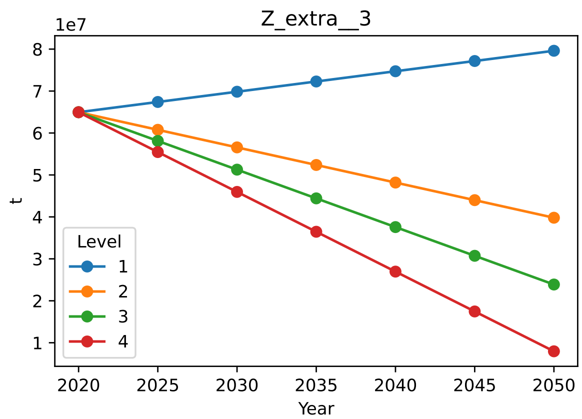
(a) Benzene



(b) Toluene



(c) Xylenes



(d) MethylAlcohol

Figure 10.1: `extra_demand` parameter data

Part III

Petrochemical production levers

11 ethylene_methanol_capacity

Lever ID ethylene_methanol_capacity
Description Increase capacity to produce ethylene and propylene from methyl alcohol
Levels

- *Level 1:* Baseline MTO capacity
- *Level 2:* Reference projected MTO capacity
- *Level 3:* 3x greater growth in capacity than the reference projected capacity
- *Level 4:* 6x greater growth in capacity than the reference projected capacity

This lever controls the available capacity of MTO (Methanol-to-Olefins), measured by the ethylene production capacity.

Currently, this is a route with small capacity, and the *Baseline* level assumes this remains constant.

The reference projection is based on the trend from Methanol Institute (2023).

Since this is currently a route with limited capacity, further hypothetical levels were added reflecting greater growth rates, to allow exploration of what would happen if this route made a larger contribution in future.

11.1 Parameter data

Figure 11.1 shows the value over time of each parameter affected by this lever.

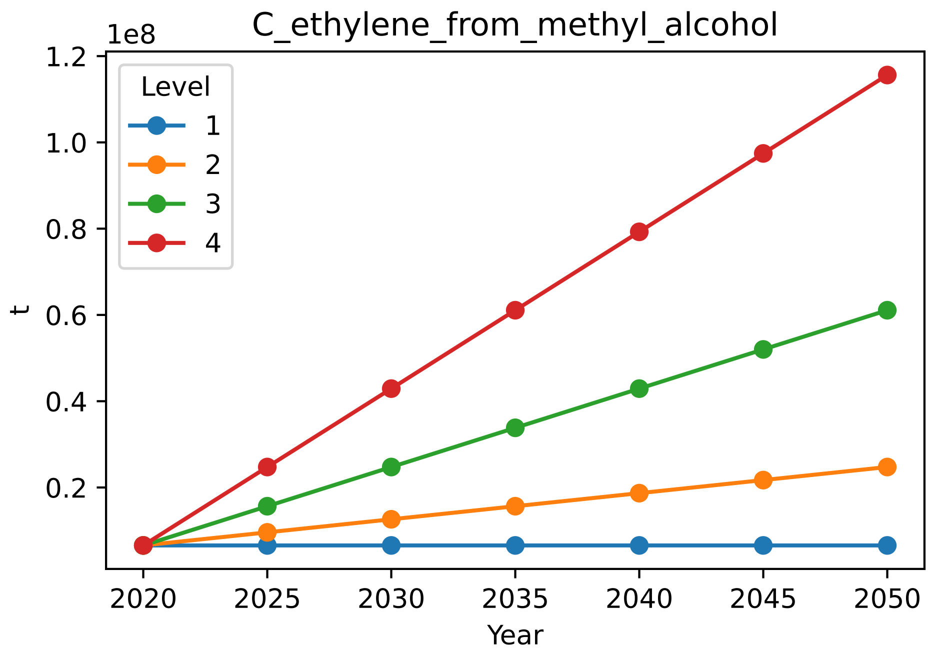


Figure 11.1: `ethylene_methanol_capacity` parameter data

12 xylenes_methyl_alcohol_capacity

Lever ID xylenes_methyl_alcohol_capacity
Description Increase capacity to produce BTX from methyl alcohol
Levels

- *Level 1:* Baseline MTA capacity
- *Level 2:* Reference projected MTA capacity
- *Level 3:* 10x greater growth in capacity than the reference projected capacity
- *Level 4:* 20x greater growth in capacity than the reference projected capacity

This lever controls the available capacity for producing BTX from methyl alcohol ("Methanol-to-aromatics", or MTA), measured by the Xylene production capacity.

The MTA process is demonstration level, according to Pales et al. (2018a).

Capacities are estimated based on data from Pales et al. (2018b), who reported projections for MTA and MTO together. They reported capacity will peak by 2030 and then decline, due to decline in coal-based methanol after 2030. However, we assume MTO/MTA capacity will continue to grow due to the emergence of renewable methanol, which is expected to be cost-competitive by 2050 given the right policies (IRENA and Institute 2021). Using only the increasing trend from Pales et al. (2018b) to project MTO/MTA growth to 2050 and then subtracting the projected MTO growth (see Chapter 11), we obtained the MTA growth. The values are comparable in magnitude to the existing size of the MTA demonstration plants reported by Wang et al. (2023).

Since this is currently a route with limited capacity, further hypothetical levels were added reflecting greater growth rates, to allow exploration of what would happen if this route made a larger contribution in future.

12.1 Parameter data

Figure 12.1 shows the value over time of each parameter affected by this lever.

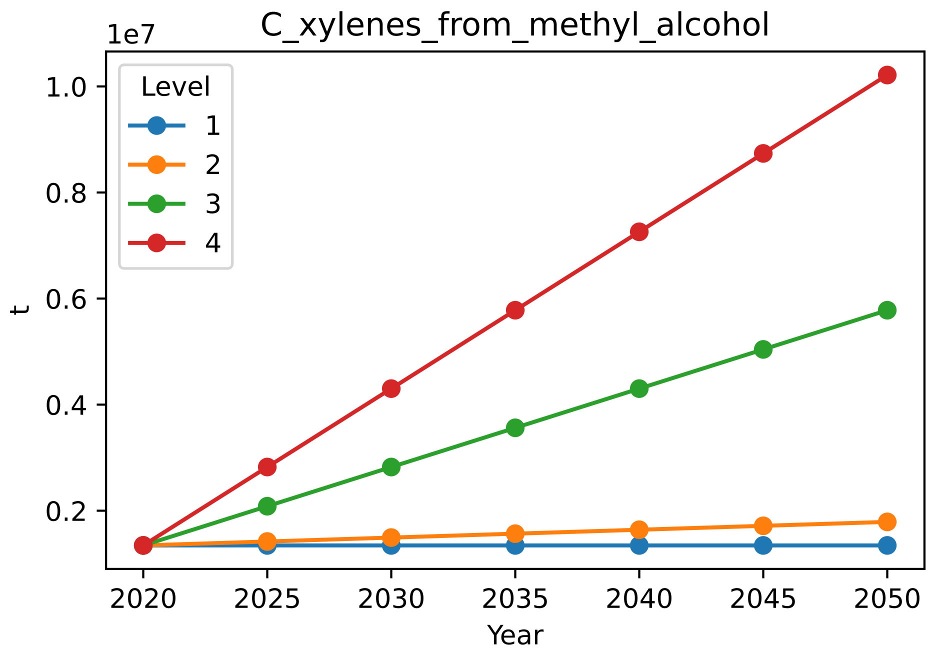


Figure 12.1: `xylenes_methyl_alcohol_capacity` parameter data

13 bioethanol_capacity

Lever ID bioethanol_capacity
Description Increase capacity for producing ethyl alcohol from bio-based feedstocks.
Levels

- *Level 1:* Baseline bioethanol capacity for ethylene production
- *Level 2:* Reference projected bioethanol capacity for ethylene production
- *Level 3:* 2x greater growth in capacity than the reference projected capacity
- *Level 4:* 4x greater growth in capacity than the reference projected capacity

This lever controls the available capacity for producing ethylene from bio-ethyl-alcohol, measured by the ethyl alcohol production capacity.

Baseline total bioethanol production is reported by OPEC (2022) and agrees well with DOE (2022) (3% difference). Of this, the majority is used as fuel, with 0.3% used for ethylene production (Mohsenzadeh, Zamani, and Taherzadeh 2017). This gives the baseline bioethylene capacity.

In the absence of specific projections for growth in bioethanol-to-ethylene capacity, we estimate 'order-of-magnitude' possible growth in this route by taking projected growth in total bioethanol and dedicating it to increasing chemicals production rather than increasing supply of ethanol for fuel. This gives a similar result to increasing the share of total bioethanol used for chemicals from 0.3% to 50% in 2050. Forecast production of fuel ethanol from 2020 to 2050 was obtained from OPEC (2022).

Since the quantity of bioethanol in this scenario is still small compared to potential demand for ethylene, we added additional hypothetical levels of capacity to explore the effect of dedicating very large amounts of biomass to this route.

13.1 Parameter data

Figure 13.1 shows the value over time of each parameter affected by this lever.

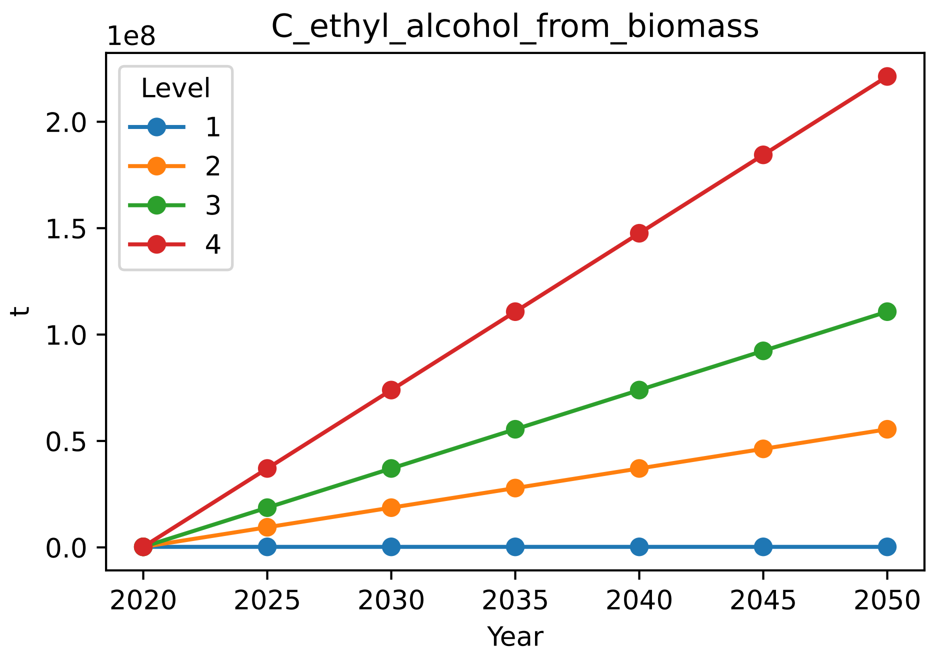


Figure 13.1: `bioethanol_capacity` parameter data

14 biosyngas_capacity

Lever ID biosyngas_capacity
Description Increase capacity for producing syngas from biomass gasification.
Levels

- *Level 1:* Baseline capacity
- *Level 2:* 50% of projected growth in biomass for bioethanol used for syngas
- *Level 3:* 100% of projected growth in biomass for bioethanol used for syngas
- *Level 4:* 200% of projected growth in biomass for bioethanol used for syngas

This lever controls the available capacity for producing syngas from biomass via gasification, measured by the syngas production capacity.

Based on figures from Barton (2021), global capacity for syngas production from biomass is about 1.3 Mt/year and 94 Mt/year from "other" sources that is assumed to be wastes gasified in a similar way to biomass. However, only a fraction of this syngas is for chemical production (largely methanol and ammonia). Production of methanol from biomass is only 0.2 Mt/year (IRENA and Institute 2021), requiring about 0.3 Mt/year syngas. Syngas for ammonia is largely out of scope of this model as fertiliser production and emissions are accounted for separately, although some ammonia synthesis is included for non-fertiliser uses downstream. The baseline bio-syngas capacity is therefore taken as 1.3 Mt/year.

In the absence of specific projections for growth in this route, further levels are extrapolated to explore the potential role of biosyngas in the wider system. The potential growth in biomass consumption is derived from the projections made from bioethanol (see Chapter 13), adjusting for the significantly higher yield of syngas than ethanol per unit mass of biomass.

14.1 Parameter data

Figure 14.1 shows the value over time of each parameter affected by this lever.

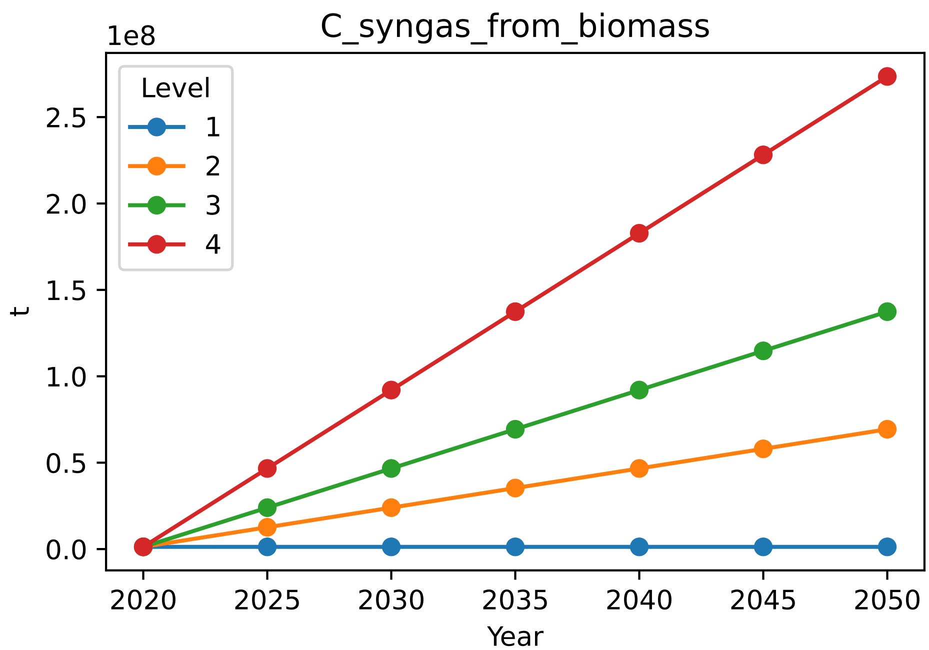


Figure 14.1: `biosyngas_capacity` parameter data

15 frac_of_biomass_feedstock

Lever ID frac_of_biomass_feedstock
Description Shift biomass feedstocks from food crops to crop residues
Levels

- *Level 1:* Baseline biomass feedstock fraction
- *Level 4:* Reference projected biomass feedstock fraction

This lever controls the mix of biomass sources used when producing bioethanol and biosyngas.

Currently about two-thirds of bioethanol comes from starch-based biomass (maize) with the rest from sugar-based biomass (sugarcane) [doe_global_2022]. Accounting for the ethanol yield from each biomass feedstock gives a baseline share of 72% ethanol from maize, 28% from sugarcane.

Historical global production of sugar cane, maize, [paddy] rice, and wheat were obtained from FAO (2024), and the trendlines were used to project production of each crop from 2020 to 2050. Using typical sugarcane bagasse to sugarcane ratio by Nikodinovic-Runic et al. (2013), corn stover to maize ratio by Ruan et al. (2019), rice straw to paddy rice ratio by irri_value_2018, and wheat straw to wheat ratio by Song et al. (2013), corresponding production of these residues can also be estimated from 2020 to 2050.

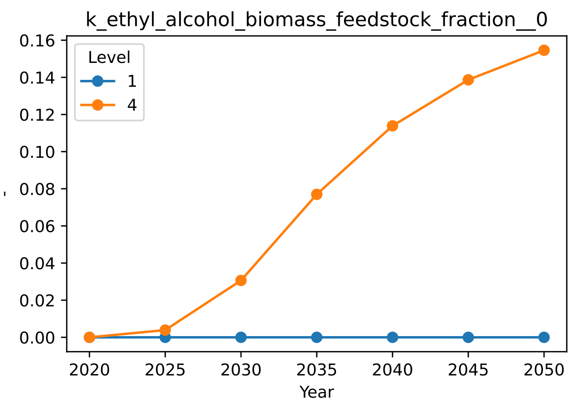
The fraction of the biomass available for ethanol production is 26% of the total sugar cane production and 14% of the total maize production using the data from Intelligence (2019) and USDA (2023), respectively. Similar to the work of Meng et al. (2023), 20% of the total crop residues produced are assumed to be available for chemical production.

In future the balance of ethanol from edible sugars versus lignocellulosic biomass is expected to shift. Lash et al. (2022) projected the future contributions of these to total fuel from 2020 to 2050, which is assumed to also apply to ethanol for chemicals. Together, after adjusting for ethanol yields, these give the projected shares of biomass contributing to bioethanol.

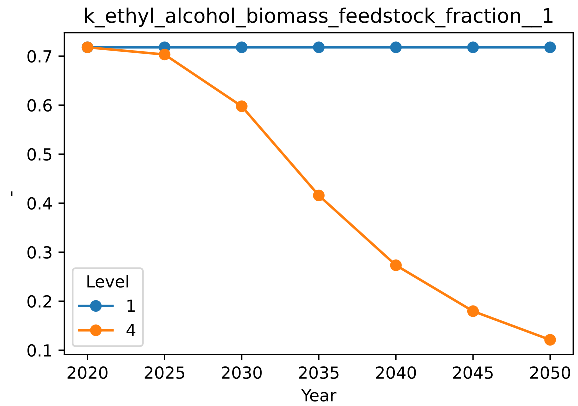
Feedstock shares used for biosyngas are assumed to be the same as for the lignocellulosic biomass used for bioethanol.

15.1 Parameter data

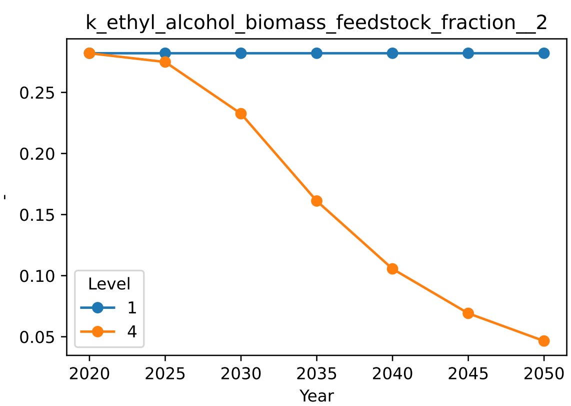
Figure 15.1 and Figure 15.2 show the value over time of each parameter affected by this lever.



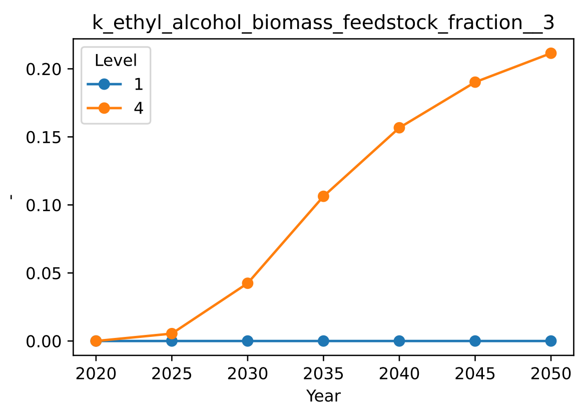
(a) CornStover



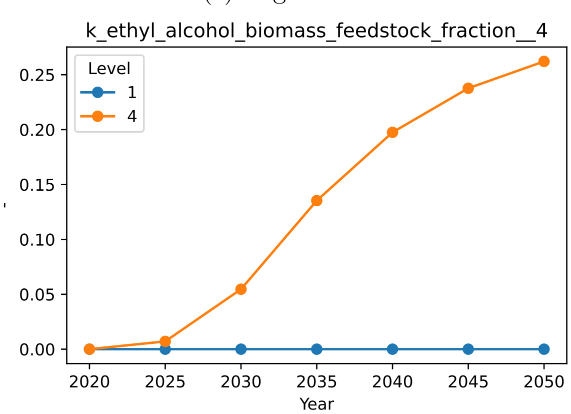
(b) Maize



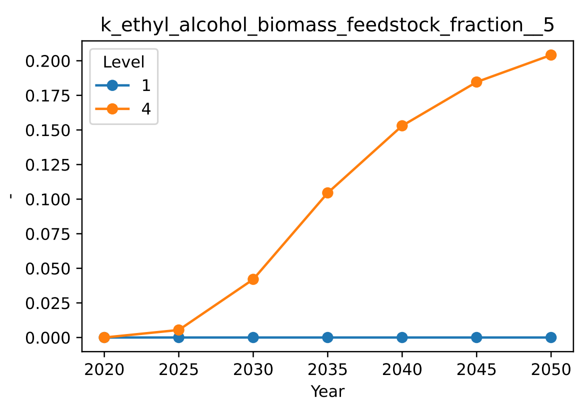
(c) Sugarcane



(d) SugarcaneBagasse

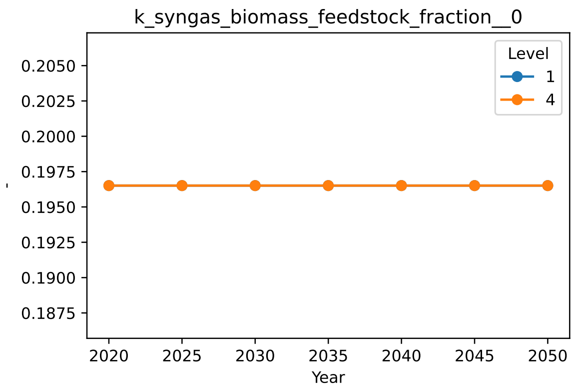


(e) WheatStraw

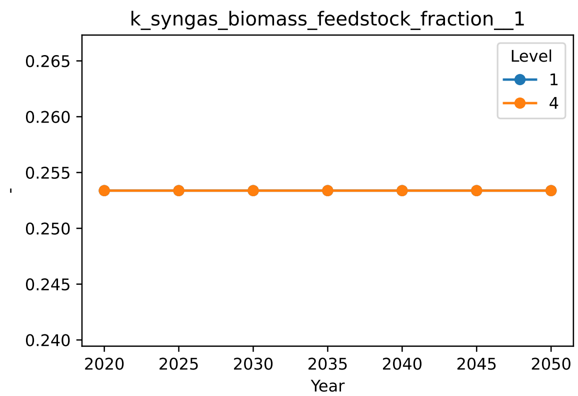


(f) RiceStraw

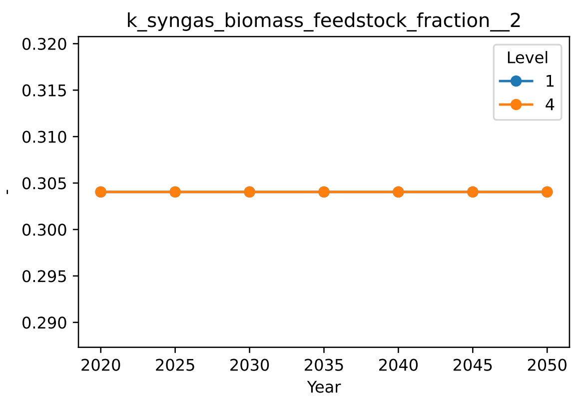
Figure 15.1: `frac_of_biomass_feedstock` parameter data (ethyl alcohol feedstocks)



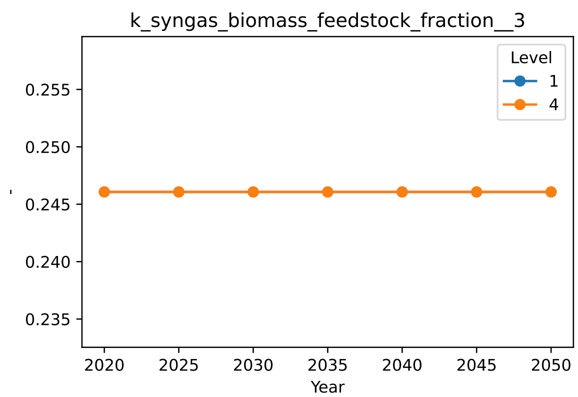
(a) CornStover



(b) SugarcaneBagasse



(c) WheatStraw



(d) RiceStraw

Figure 15.2: `frac_of_biomass_feedstock` parameter data (bio-syngas feedstocks)

16 olefins_paraffins_mix

Lever ID olefins_paraffins_mix

Description Determines the mix of paraffins (i.e., naptha, ethane) from which olefins are produced. Most of the regions in the world produce olefins from naphtha while some produce olefins from ethane.

Levels

- *Level 1:* Baseline fraction of ethane
- *Level 2:* Replace ethane use with naphtha

This lever controls the split of ethane vs naphtha as the feedstock for fossil production of olefins via steam cracking. It is intended to reflect the geographical split of demand into regions that have each feedstock available.

The baseline shares were derived from data on steam cracker feeds from ICIS (2021). Our model has only two representative varieties of steam cracker, from ethane and naphtha feedstocks, so the ICIS data was aggregated into lighter and heavier feeds, giving a baseline fraction of 46% of ethylene from ethane. This is slightly higher than the share of 39% for lighter-feed steam cracking reported for 2017 by Pales et al. (2018b).

To explore what effect shifts in feedstock have on the overall system, an additional level was added representing a shift towards naphtha.

16.1 Parameter data

Figure 16.1 shows the value over time of each parameter affected by this lever.

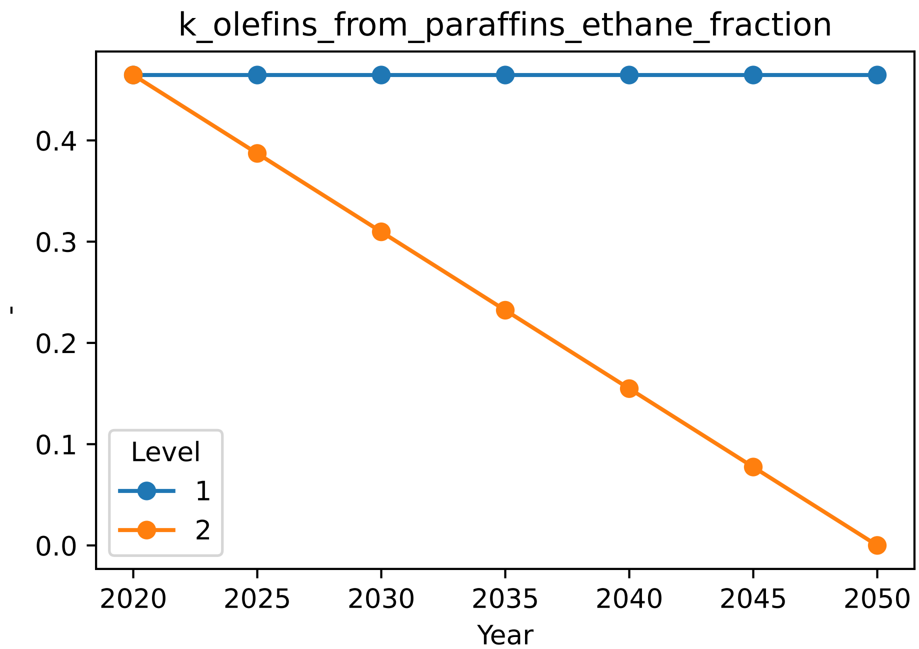


Figure 16.1: `olefins_paraffins_mix` parameter data

Part IV

Hydrogen levers

17 green_hydrogen_capacity

Lever ID green_hydrogen_capacity
Description Sets the total capacity to produce "green" hydrogen via water electrolysis using low-carbon electricity
Levels

- *Level 1:* Baseline green hydrogen capacity
- *Level 2:* Growth in capacity according to McKinsey "Fading momentum" scenario
- *Level 3:* Growth in capacity according to McKinsey "Achieved commitments" scenario
- *Level 4:* Hypothetical further doubling in green hydrogen capacity for chemicals, to allow all hydrogen demand to be supplied by this route

This lever controls production capacity for "green" hydrogen, i.e. from water electrolysis.

Currently this route is not used, so the baseline capacity remains at zero.

Growth scenarios are based on the hydrogen outlook by Gulli et al. (2024). They projected total "clean hydrogen" (i.e. including green and blue) capacity in different scenarios, as well as the amount of hydrogen used by the chemical sector in 2035 and 2050. This is used to estimate the fraction of all hydrogen projection which is used by the chemical sector in each scenario, which ranges from 18% (highest growth in hydrogen, in 2050) to 53% (lowest growth, in 2035).

These fractions of capacity used for the chemical sector are assumed to apply to the green and blue hydrogen capacity available in each scenario, leading to the capacity levels set by this lever.

The maximum capacity found this way is 54 Mt/year in 2050, which is insufficient to supply all potential demand for hydrogen in the model. To allow exploration of scenarios fully supplied by green hydrogen, an additional "full hydrogen" level was added with greater hypothetical capacity.

17.1 Parameter data

Figure 17.1 shows the value over time of each parameter affected by this lever.

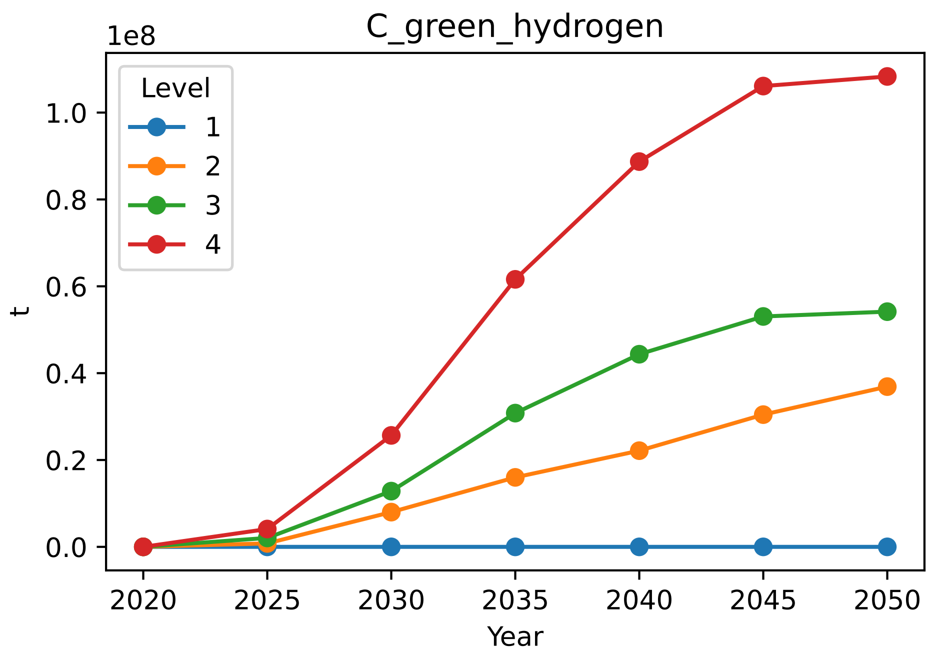


Figure 17.1: `green_hydrogen_capacity` parameter data

18 blue_hydrogen_capacity

Lever ID blue_hydrogen_capacity
Description Sets the total capacity to produce "blue" hydrogen via natural gas steam methane reforming with CCS
Levels

- *Level 1:* Baseline blue hydrogen capacity
- *Level 2:* Growth in capacity according to McKinsey "Fading momentum" scenario
- *Level 3:* Growth in capacity according to McKinsey "Achieved commitments" scenario

This lever controls production capacity for "blue" hydrogen, i.e. from steam methane reforming of natural gas, with carbon capture and storage (CCS).

The values were derived as described in Chapter 17.

18.1 Parameter data

Figure 18.1 shows the value over time of each parameter affected by this lever.

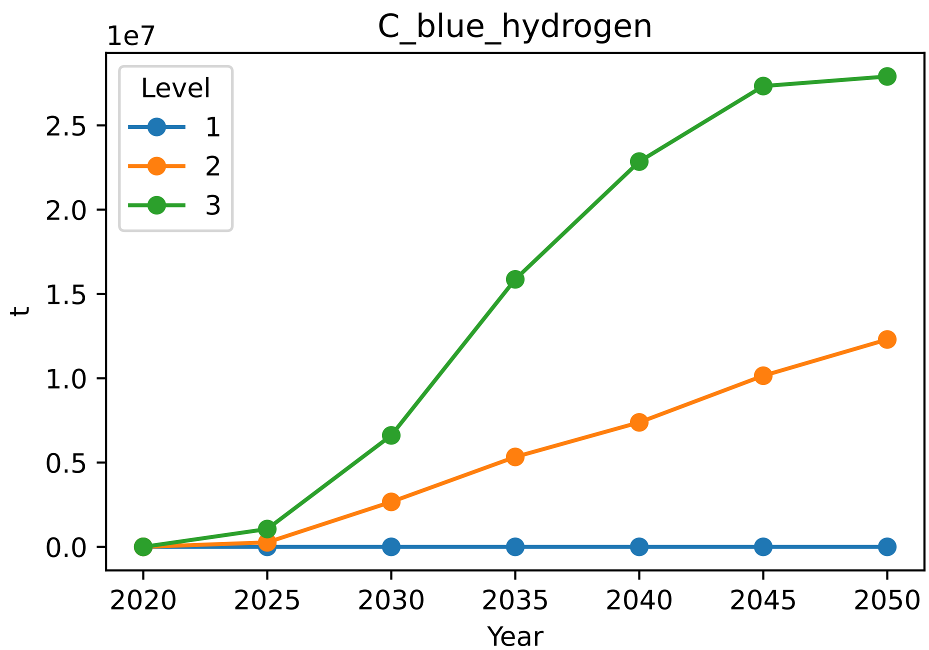


Figure 18.1: `blue_hydrogen_capacity` parameter data

Part V

Abatement levers

19 ccs_incineration

Lever ID ccs_incineration
Description Level of emissions abatement on incineration emissions
Levels

- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

This lever controls the level of emissions abatement on end-of-life incineration.

Currently practically no CCS is in use (Meng et al. 2023), so the baseline level has no capacity applied.

To allow exploring different levels of CCS applied to incineration emissions specifically, hypothetical higher levels are included.

19.1 Parameter data

Figure 19.1 shows the value over time of each parameter affected by this lever.

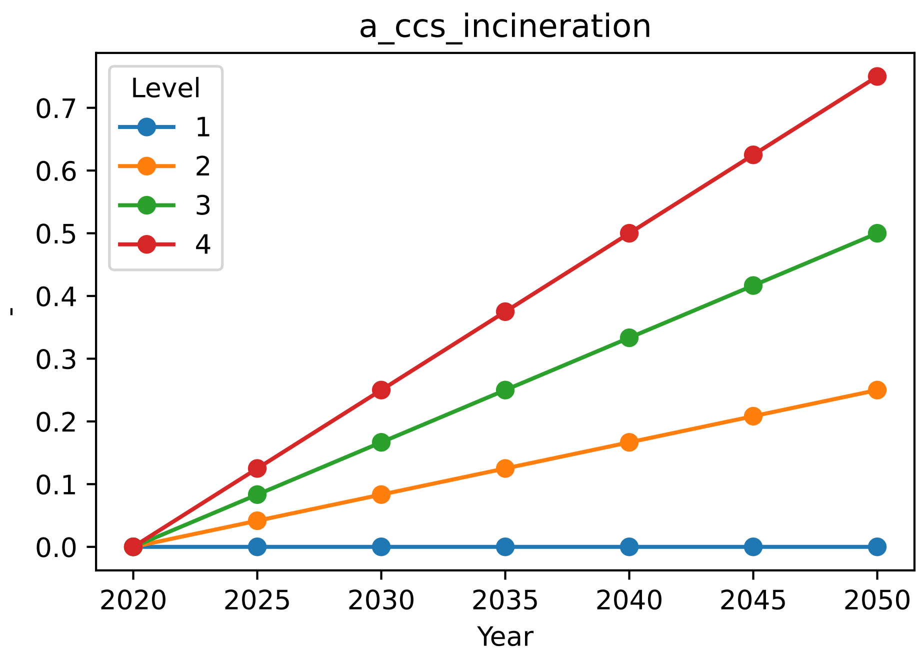


Figure 19.1: `ccs_incineration` parameter data

20 ccs_process_emissions

Lever ID ccs_process_emissions
Description Level of emissions abatement on process emissions (excluding incineration)
Levels

- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

This lever controls the level of emissions abatement on process emissions (excluding end-of-life incineration).

Currently practically no CCS is in use (Meng et al. 2023), so the baseline level has no capacity applied.

To allow exploring different levels of CCS applied to production process emissions specifically, hypothetical higher levels are included.

20.1 Parameter data

Figure 20.1 shows the value over time of each parameter affected by this lever.

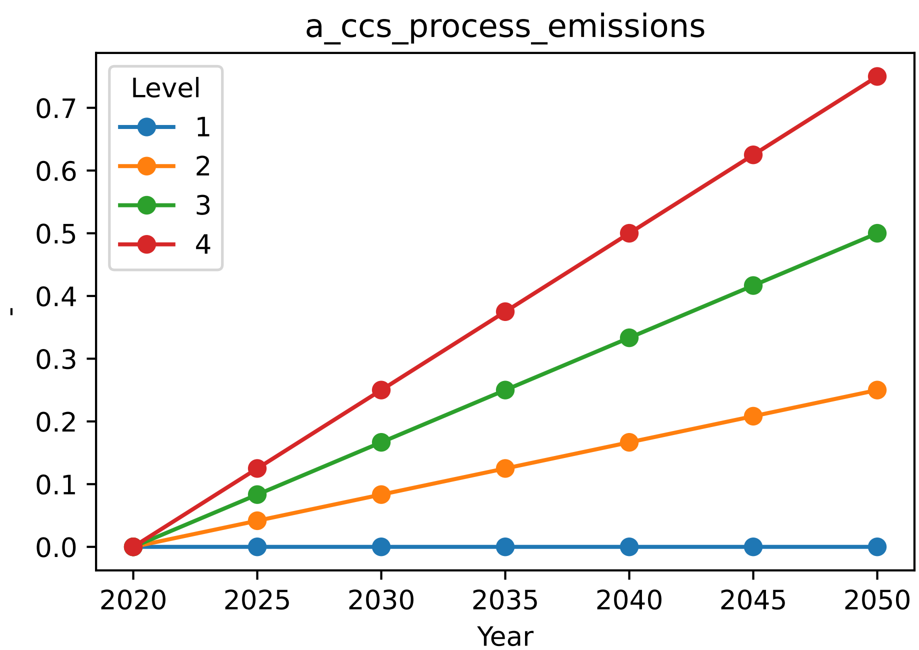


Figure 20.1: `ccs_process_emissions` parameter data

21 ccs_utility_combustion

Lever ID ccs_utility_combustion
Description Level of emissions abatement on combustion of natural gas utility
Levels

- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

This lever controls the level of emissions abatement on utility combustion emissions.

Currently practically no CCS is in use (Meng et al. 2023), so the baseline level has no capacity applied.

To allow exploring different levels of CCS applied to combustion emissions specifically, hypothetical higher levels are included.

21.1 Parameter data

Figure 21.1 shows the value over time of each parameter affected by this lever.

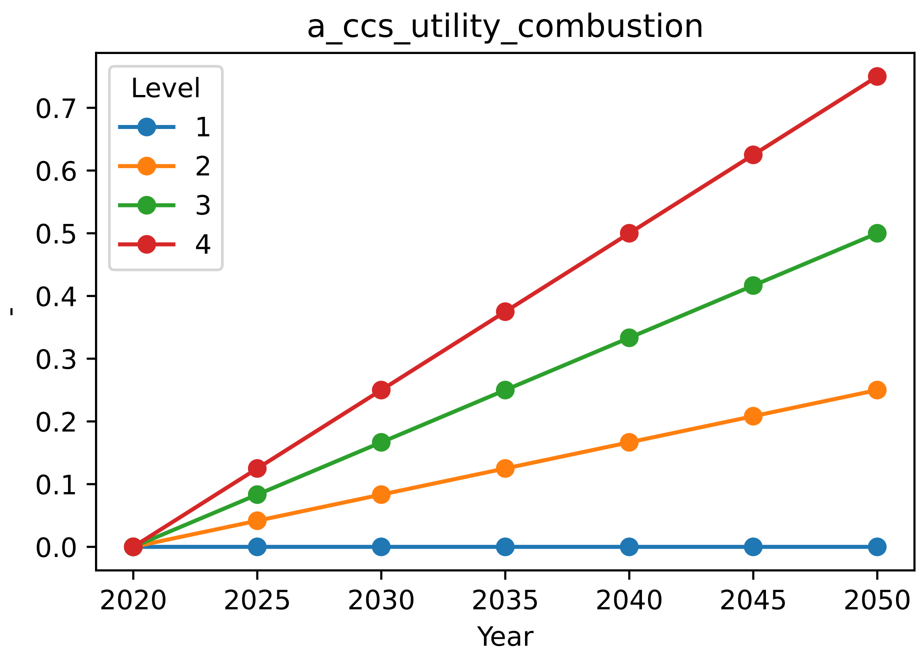


Figure 21.1: `ccs_utility_combustion` parameter data

Part VI

Utilities & emissions data

22 electricity_requirements

Lever ID electricity_requirements
Description
Levels

- *Level 1:* Baseline/constant

This lever sets the baseline values for electricity utility requirements for all processes.

Data was sourced from Zhao, Jiang, and Wang (2021), Jiang et al. (2020), Rosental, Fröhlich, and Liebich (2020), Oni et al. (2022), IEA (2021), and cross-checked against data from Markit (2021) to estimate indicative electricity requirements for each process.

22.1 Parameter data

Table 22.1 shows parameter values for process electricity requirements.

Table 22.1: `electricity_requirements` parameter data. Values in kWh per tonne product.

Parameter	Level 1	Units
ElecReq_AceticAcidSynthesis	90	kWh/t
ElecReq_AcrylonitrileSynthesis	300	kWh/t
ElecReq_AdipicAcidSynthesis	100	kWh/t
ElecReq_CarbonDioxideHydrogenationToMethylAlcohol	330	kWh/t
ElecReq_CatalyticReformingOfNaphthaForToluene	240	kWh/t
ElecReq_CatalyticReformingOfNaphthaForXylenes	600	kWh/t
ElecReq_ChemicalRecyclingOfMixedPolymersAtEOL	1200	kWh/t
ElecReq_CoalGasificationToSyngas	277	kWh/t
ElecReq_CornStoverGasificationToSyngas	185	kWh/t
ElecReq_CyclohexaneSynthesis	70	kWh/t
ElecReq_DealkylationOfTolueneForBenzene	80	kWh/t
ElecReq_DehydrationOfEthylAlcohol	400	kWh/t
ElecReq_DehydrogenationOfButaneForButadiene	300	kWh/t
ElecReq_DehydrogenationOfPropane	1200	kWh/t
ElecReq_DisproportionationOfTolueneForXylenes	65	kWh/t
ElecReq_DistillationOfButylenesForButadiene	120	kWh/t

Table 22.1: `electricity_requirements` parameter data. Values in kWh per tonne product.

Parameter	Level 1	Units
ElecReq_DistillationOfPyrolysisGasolineForBTX	17	kWh/t
ElecReq_EthylAlcoholSynthesisFromCornStover	350	kWh/t
ElecReq_EthylAlcoholSynthesisFromMaize	530	kWh/t
ElecReq_EthylAlcoholSynthesisFromRiceStraw	300	kWh/t
ElecReq_EthylAlcoholSynthesisFromSugarcane	110	kWh/t
ElecReq_EthylAlcoholSynthesisFromSugarcaneBagasse	430	kWh/t
ElecReq_EthylAlcoholSynthesisFromWheatStraw	270	kWh/t
ElecReq_EthyleneGlycolSynthesis	150	kWh/t
ElecReq_EthyleneOxideSynthesis	600	kWh/t
ElecReq_FischerTropschSynthesisOfOlefinsFromSyngas	6000	kWh/t
ElecReq_FluidCatalyticCrackingOfGasOil	1000	kWh/t
ElecReq_HexamethylenediamineSynthesisFromButadiene	360	kWh/t
ElecReq_HydrogenCyanideSynthesis	600	kWh/t
ElecReq_IsophthalicAcidSynthesis	500	kWh/t
ElecReq_MechanicalRecyclingOfFibrePPAAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfHDPEPolyethyleneAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfLDPEPolyethyleneAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfLLDPEAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfPETPolyethyleneTerephthalatePolyestersAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfPPPolypropyleneAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfPSPolystyreneAtEOL	200	kWh/t
ElecReq_MechanicalRecyclingOfPVCPolyvinylChlorideAtEOL	200	kWh/t
ElecReq_MethylAlcoholSynthesis	20	kWh/t
ElecReq_MethylAlcoholToAromatics	580	kWh/t
ElecReq_MethylAlcoholToOlefins	35	kWh/t
ElecReq_MethylAlcoholToPropylene	250	kWh/t
ElecReq_NaturalGasSteamMethaneReformingToHydrogen	960	kWh/t
ElecReq_NaturalGasSteamMethaneReformingToSyngas	75.3	kWh/t
ElecReq_NaturalGasSteamMethaneReformingWithCCSToHydrogen	4420	kWh/t
ElecReq_OtherOrganicChemicalsSynthesis	240	kWh/t
ElecReq_PolymerisationOfFibrePPA	550	kWh/t
ElecReq_PolymerisationOfHDPE	400	kWh/t
ElecReq_PolymerisationOfLDPE	1000	kWh/t
ElecReq_PolymerisationOfLLDPE	260	kWh/t
ElecReq_PolymerisationOfOtherPolymers	300	kWh/t
ElecReq_PolymerisationOfPET	17	kWh/t
ElecReq_PolymerisationOfPP	500	kWh/t
ElecReq_PolymerisationOfPUR	120	kWh/t
ElecReq_PolymerisationOfPVC	110	kWh/t

Table 22.1: `electricity_requirements` parameter data. Values in kWh per tonne product.

Parameter	Level 1	Units
ElecReq_PolymerisationOfPolystyrene	40	kWh/t
ElecReq_PolymerisationOfStyreneButadiene	1100	kWh/t
ElecReq_PolyolsSynthesis	55	kWh/t
ElecReq_PropyleneOxideSynthesis	200	kWh/t
ElecReq_RiceStrawGasificationToSyngas	185	kWh/t
ElecReq_SodiumChlorideElectrolysisForChlorine	3000	kWh/t
ElecReq_SteamCrackingOfEthane	13	kWh/t
ElecReq_SteamCrackingOfNaphtha	60	kWh/t
ElecReq_StyreneSynthesis	81	kWh/t
ElecReq_SugarCaneBagasseGasificationToSyngas	185	kWh/t
ElecReq_SyngasToAmmoniaProduction	336	kWh/t
ElecReq_TerephthalicAcidSynthesis	80	kWh/t
ElecReq_TolueneDiisocyanateSynthesis	240	kWh/t
ElecReq_VinylChlorideSynthesis	140	kWh/t
ElecReq_WaterElectrolysisForHydrogen	53830	kWh/t
ElecReq_WheatStrawGasificationToSyngas	185	kWh/t

23 natural_gas_requirements

Lever ID natural_gas_requirements
Description
Levels

- *Level 1:* Baseline/constant

This lever sets the baseline values for natural gas utility requirements for all processes.

Data was sourced from Zhao, Jiang, and Wang (2021), Jiang et al. (2020), Rosental, Fröhlich, and Liebich (2020), Oni et al. (2022), IEA (2021), and cross-checked against data from Markit (2021) to estimate indicative natural gas requirements for each process.

Where steam utility requirements were known for processes, these were converted into equivalent natural gas requirements to better indicate the total energy requirements of the process.

23.1 Parameter data

Table 23.1 shows parameter values for natural gas utility requirements.

Table 23.1: `natural_gas_requirements` parameter data. Values in MJ per tonne product.

Parameter	Level 1	Units
NGReq_AceticAcidSynthesis	2200	MJ/t
NGReq_AcrylonitrileSynthesis	11000	MJ/t
NGReq_AdipicAcidSynthesis	37000	MJ/t
NGReq_CarbonDioxideHydrogenationToMethylAlcohol	0	MJ/t
NGReq_CatalyticReformingOfNaphthaForToluene	21000	MJ/t
NGReq_CatalyticReformingOfNaphthaForXylenes	18000	MJ/t
NGReq_ChemicalRecyclingOfMixedPolymersAtEOL	9800	MJ/t
NGReq_CoalGasificationToSyngas	0	MJ/t
NGReq_CornStoverGasificationToSyngas	0	MJ/t
NGReq_CyclohexaneSynthesis	0	MJ/t
NGReq_DealkylationOfTolueneForBenzene	2600	MJ/t
NGReq_DehydrationOfEthylAlcohol	8500	MJ/t
NGReq_DehydrogenationOfButaneForButadiene	23000	MJ/t

Table 23.1: `natural_gas_requirements` parameter data. Values in MJ per tonne product.

Parameter	Level 1	Units
NGReq__DehydrogenationOfPropane	8500	MJ/t
NGReq__DisproportionationOfTolueneForXylenes	14000	MJ/t
NGReq__DistillationOfButylenesForButadiene	4300	MJ/t
NGReq__DistillationOfPyrolysisGasolineForBTX	9400	MJ/t
NGReq__EthylAlcoholSynthesisFromCornStover	46000	MJ/t
NGReq__EthylAlcoholSynthesisFromMaize	16000	MJ/t
NGReq__EthylAlcoholSynthesisFromRiceStraw	0	MJ/t
NGReq__EthylAlcoholSynthesisFromSugarcane	0	MJ/t
NGReq__EthylAlcoholSynthesisFromSugarcaneBagasse	25000	MJ/t
NGReq__EthylAlcoholSynthesisFromWheatStraw	0	MJ/t
NGReq__EthyleneGlycolSynthesis	9600	MJ/t
NGReq__EthyleneOxideSynthesis	0	MJ/t
NGReq__FischerTropschSynthesisOfOlefinsFromSyngas	38000	MJ/t
NGReq__FluidCatalyticCrackingOfGasOil	4300	MJ/t
NGReq__HexamethylenediamineSynthesisFromButadiene	25000	MJ/t
NGReq__HydrogenCyanideSynthesis	0	MJ/t
NGReq__IsophthalicAcidSynthesis	9500	MJ/t
NGReq__MechanicalRecyclingOfFibrePPAAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfHDPEPolyethyleneAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfLDPEPolyethyleneAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfLLDPEAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfPETPolyethyleneTerephthalatePolyestersAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfPPPolypropyleneAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfPSPolystyreneAtEOL	0	MJ/t
NGReq__MechanicalRecyclingOfPVCPolyvinylChlorideAtEOL	0	MJ/t
NGReq__MethylAlcoholSynthesis	450	MJ/t
NGReq__MethylAlcoholToAromatics	2275	MJ/t
NGReq__MethylAlcoholToOlefins	8900	MJ/t
NGReq__MethylAlcoholToPropylene	14000	MJ/t
NGReq__NaturalGasSteamMethaneReformingToHydrogen	60	MJ/t
NGReq__NaturalGasSteamMethaneReformingToSyngas	0	MJ/t
NGReq__NaturalGasSteamMethaneReformingWithCCSToHydrogen	130	MJ/t
NGReq__OtherOrganicChemicalsSynthesis	13000	MJ/t
NGReq__PolymerisationOfFibrePPA	1800	MJ/t
NGReq__PolymerisationOfHDPE	0	MJ/t
NGReq__PolymerisationOfLDPE	430	MJ/t
NGReq__PolymerisationOfLLDPE	0	MJ/t
NGReq__PolymerisationOfOtherPolymers	620	MJ/t
NGReq__PolymerisationOfPET	2900	MJ/t

Table 23.1: `natural_gas_requirements` parameter data. Values in MJ per tonne product.

Parameter	Level 1	Units
NGReq_PolymerisationOfPP	1200	MJ/t
NGReq_PolymerisationOfPUR	0	MJ/t
NGReq_PolymerisationOfPVC	1400	MJ/t
NGReq_PolymerisationOfPolystyrene	51	MJ/t
NGReq_PolymerisationOfStyreneButadiene	12000	MJ/t
NGReq_PolyolsSynthesis	1100	MJ/t
NGReq_PropyleneOxideSynthesis	36000	MJ/t
NGReq_RiceStrawGasificationToSyngas	0	MJ/t
NGReq_SodiumChlorideElectrolysisForChlorine	9000	MJ/t
NGReq_SteamCrackingOfEthane	14000	MJ/t
NGReq_SteamCrackingOfNaphtha	21000	MJ/t
NGReq_StyreneSynthesis	9000	MJ/t
NGReq_SugarCaneBagasseGasificationToSyngas	0	MJ/t
NGReq_SyngasToAmmoniaProduction	0	MJ/t
NGReq_TerephthalicAcidSynthesis	9000	MJ/t
NGReq_TolueneDiisocyanateSynthesis	40000	MJ/t
NGReq_VinylChlorideSynthesis	4700	MJ/t
NGReq_WaterElectrolysisForHydrogen	0	MJ/t
NGReq_WheatStrawGasificationToSyngas	0	MJ/t

24 electricity_emission_factor

Lever ID electricity_emission_factor
Description Reduce emissions of electricity drawn from the grid
Levels

- *Level 1:* No improvement from today
- *Level 2:* Global grid intensity reaches current North American levels
- *Level 3:* Level based on Paris Agreement NDCs
- *Level 4:* Near decarbonisation of electricity

This lever controls the emissions factor for grid electricity production.

A range of levels is provided, from current global average to the low value for wind energy used by Meys et al. (2021) in their plastics decarbonisation scenarios.

24.1 Parameter data

Figure 24.1 shows the value over time of each parameter affected by this lever.

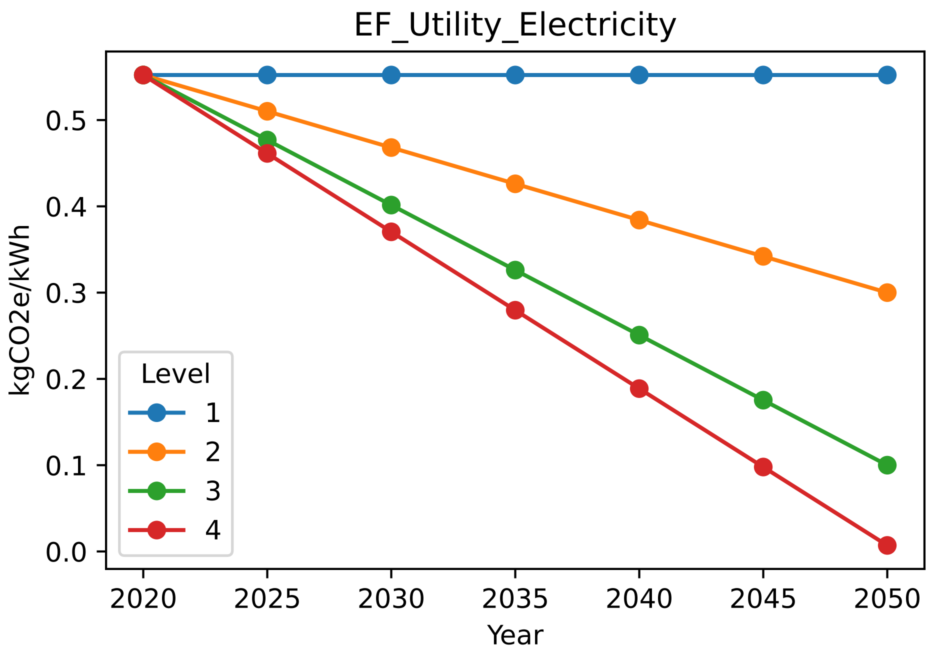


Figure 24.1: `electricity_emission_factor` parameter data

25 natural_gas_emission_factor

Lever ID natural_gas_emission_factor
Description Emission factor of natural gas when it is combusted on-site for power and/or steam generation
Levels

- *Level 1:* Baseline/constant

This lever controls the emissions factor for natural gas combustion as a utility.

The value is based on DESNZ and DEFRA (2023) scope 1 emissions factors.

25.1 Parameter data

Figure 25.1 shows the value over time of each parameter affected by this lever.

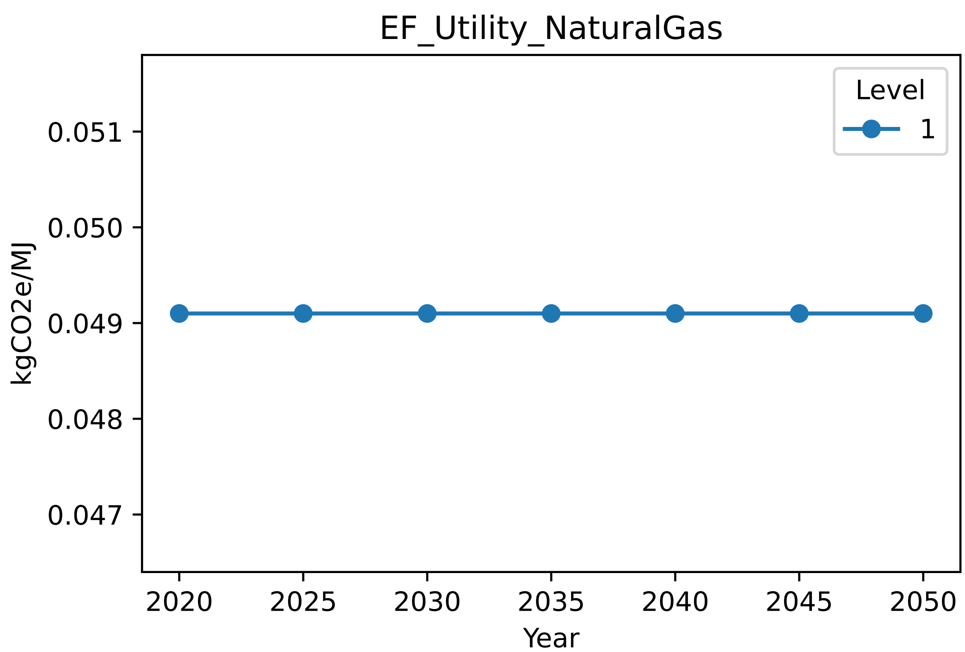


Figure 25.1: `natural_gas_emission_factor` parameter data

26 direct_process_emissions

Lever ID direct_process_emissions
Description Direct process emissions of steam cracking, methyl alcohol synthesis, adipic acid acid synthesis, and ethylene oxide synthesis; these four need to be monitored due to their process emissions
Levels

- *Level 1:* Basline/constant

This lever sets the baseline direct process emissions from reactions and internal non-utility combustion (consistent with the IPCC definition).

The default direct process emissions from the IPCC guidelines (Harnisch et al. 2006) were used as a starting point, unless modifications were needed as described below.

26.1 Process emissions

Steam cracking has significant CO_2 emissions from combustion, as described by the IPCC emissions factors, but these are already accounted for by utility energy inputs in our model, so are reported as utility emissions rather than direct process emissions. CH_4 emissions are calculated based on IPCC emissions factor estimates.

For production of methanol, we model syngas production and methanol production as separate processes, whereas IPCC emissions factors include both steps together, and due to the integrated nature of the processes it can be difficult to allocate emissions to specific stages. Based on a carbon balance of the processes, most CO_2 comes from the syngas production stage, so IPCC emissions factors by feedstock are allocated to those processes, accounting for a 1 kg methanol yield from 1.5 kg syngas. Direct CH_4 emissions from methanol synthesis based on IPCC emissions factors are included.

Emissions factors for direct process emissions from adipic acid synthesis, ethylene oxide synthesis and acrylonitrile synthesis are used directly.

26.2 Biogenic carbon sequestration

Since the chemical sector can potentially act as a sink for carbon emissions (Meng et al. 2023) it is important to clearly model and report negative sequestered carbon from biomass feedstocks. To simplify modelling of biomass production, sequestration is modelled as happening at the point of conversion to a bio-based chemical (i.e. syngas or ethanol) rather than further upstream, based on the assumption that other biogenic carbon is released back to the atmosphere in the short term.

The carbon content of syngas is assumed to be 30% by mass, giving 1.1 kg CO_2 sequestered per kg syngas.

The carbon content of ethyl alcohol is assumed to be 52% by mass, giving 1.9 kg CO_2 sequestered per kg ethyl alcohol.

These are included as negative emissions linked to the bio-syngas and bio-ethyl-alcohol production processes.

26.3 Parameter data

Table 26.1 shows parameter values for direct process emissions.

Table 26.1: `direct_process_emissions` parameter data. Values in tonnes of GHG per tonne product.

Parameter	Level 1	Units
DirProcEmis_CH4_AcrylonitrileSynthesis	0.000	t CH4/t acrylonitrile
DirProcEmis_CH4_EthyleneOxideSynthesis	0.002	t CH4/t ethylene oxide
DirProcEmis_CH4_MethylAlcoholSynthesis	0.002	t CH4/t methyl alcohol
DirProcEmis_CH4_SteamCrackingOfEthane	0.006	t CH4/t ethylene
DirProcEmis_CH4_SteamCrackingOfNaphtha	0.003	t CH4/t ethylene
DirProcEmis_CO2_AcrylonitrileSynthesis	0.790	t CO2/t acrylonitrile
DirProcEmis_CO2_CoalGasificationToSyngas	3.513	t CO2/t syngas
DirProcEmis_CO2_CornStoverGasificationToSyngas	-1.096	t CO2/t syngas
DirProcEmis_CO2_EthylAlcoholSynthesisFromCornStover	-1.912	t CO2/t ethyl alcohol
DirProcEmis_CO2_EthylAlcoholSynthesisFromMaize	-1.912	t CO2/t ethyl alcohol
DirProcEmis_CO2_EthylAlcoholSynthesisFromRiceStraw	-1.912	t CO2/t ethyl alcohol
DirProcEmis_CO2_EthylAlcoholSynthesisFromSugarcane	-1.912	t CO2/t ethyl alcohol
DirProcEmis_CO2_EthylAlcoholSynthesisFromSugarcaneBagasse	-1.912	t CO2/t ethyl alcohol
DirProcEmis_CO2_EthylAlcoholSynthesisFromWheatStraw	-1.912	t CO2/t ethyl alcohol

Table 26.1: `direct_process_emissions` parameter data. Values in tonnes of GHG per tonne product.

Parameter	Level 1	Units
DirProcEmis_CO2_EthyleneOxideSynthesis	0.663	t CO2/t ethylene oxide
DirProcEmis_CO2_NaturalGasSteamMethaneReformingToSyngas	0.445	t CO2/t syngas
DirProcEmis_CO2_RiceStrawGasificationToSyngas	-1.096	t CO2/t syngas
DirProcEmis_CO2_SugarCaneBagasseGasificationToSyngas	-1.096	t CO2/t syngas
DirProcEmis_CO2_WheatStrawGasificationToSyngas	-1.096	t CO2/t syngas
DirProcEmis_N2O_AdipicAcidSynthesis	0.300	t N2O/t adipic acid

27 feedstock_emission_factor

Lever ID feedstock_emission_factor
Description Emission factor of the feedstocks which must account for during their extraction/production, refining, and/or transportation into the petrochemical supply chains
Levels

- *Level 1:* Baseline/constant

This lever controls the emissions factor for upstream production of the feedstocks that enter the model.

Emissions factors for natural gas, coal, gas oil, propane and butane were taken from DESNZ and DEFRA (2023) scope 3 emissions factors data.

Approximate emissions factors for naphtha and ethane supply were based on the study by Nanthachatchavankul, Gridsdanurak, and Chiarakorn (2012) for ethylene production in Thailand, which was assumed to be the mean value between reported values by Bousted (2005) (assumed minimum) and DESNZ and DEFRA (2023) (assumed maximum).

Biomass crop feedstocks are from Yuttitham, Gheewala, and Chidthaisong (2011) for sugarcane production in Thailand (assumed mean value between the reported values by Sanches et al. (2023) as the assumed minimum and Chandra et al. (2018) as the assumed maximum), and Farag et al. (2018) for corn production in Egypt (assumed mean between the reported values by Giusti et al. (2023) as the assumed minimum and Zhang et al. (2017) as the assumed maximum). Crop residues are represented by DESNZ and DEFRA (2023) scope 3 emissions for generic straw/grass biomass.

27.1 Parameter data

Table 23.1 shows parameter values for natural gas utility requirements.

Table 27.1: `feedstock_emission_factor` parameter data. Values in $kgCO_{2e}$ per tonne product.

Parameter	Level 1	Units
EF_Feedstock_Butane	344	kgCO2e/t
EF_Feedstock_Coal	418	kgCO2e/t

Table 27.1: `feedstock_emission_factor` parameter data. Values in $kgCO_{2e}$ per tonne product.

Parameter	Level 1	Units
EF_Feedstock_CornStover	69	kgCO2e/t
EF_Feedstock_Ethane	992	kgCO2e/t
EF_Feedstock_GasOil	744	kgCO2e/t
EF_Feedstock_Maize	307	kgCO2e/t
EF_Feedstock_Naphtha	501	kgCO2e/t
EF_Feedstock_NaturalGas	423	kgCO2e/t
EF_Feedstock_Propane	353	kgCO2e/t
EF_Feedstock_RiceStraw	69	kgCO2e/t
EF_Feedstock_SugarCane	45	kgCO2e/t
EF_Feedstock_SugarCaneBagasse	69	kgCO2e/t
EF_Feedstock_WheatStraw	69	kgCO2e/t

28 final_treatment_emission_factor

Lever ID final_treatment_emission_factor
Description Emission factor of the mixed polymers after they underwent the final treatment option
Levels

- *Level 1:* Baseline/constant

This lever controls the emissions factors for end-of-life final treatments.

Emissions from incineration are based on data from Vlasopoulos et al. (2023) for incineration of mixed plastic waste in Europe.

Emissions from landfilling are based on data from OECD (2022) for sanitary landfill, global scope.

According to OECD (2022), mismanaged waste is "Waste that is not captured by any state-of-the-art waste collection or treatment facilities. It includes waste that is burned in open pits, dumped into seas or open waters, or disposed of in unsanitary landfills and dumpsites." Emissions are assumed to be the average of incineration and landfilling.

28.1 Parameter data

Table 28.1 shows parameter values for emissions from final treatment processes.

Table 28.1: `final_treatment_emission_factor` parameter data. Values in tonnes of GHG per tonne product.

Parameter	Level 1	Units
DirProcEmis_CO2_Incineration	2.593	t CO2/t plastic
DirProcEmis_CO2_Landfilling	0.076	t CO2/t plastic
DirProcEmis_CO2_Mismanagement	1.335	t CO2/t plastic

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