Lever data and descriptions

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Table of contents

1 Overview of levers

These pages each present the data for each lever, with additional background data.

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 generated documentation here.

Part I

Fertilisers

3 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).

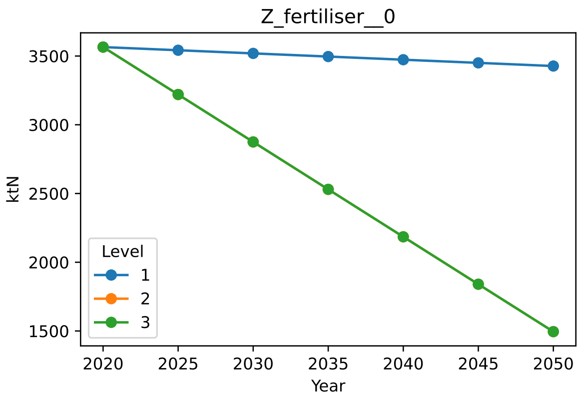
The regional total demand for synthetic nitrogen fertilisers in the BAU scenario in 2050 is extracted from the forecast made by the FAO (2022). The fractions of various nitrogen fertiliser are estimated using the regional fractions in 2019.

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.

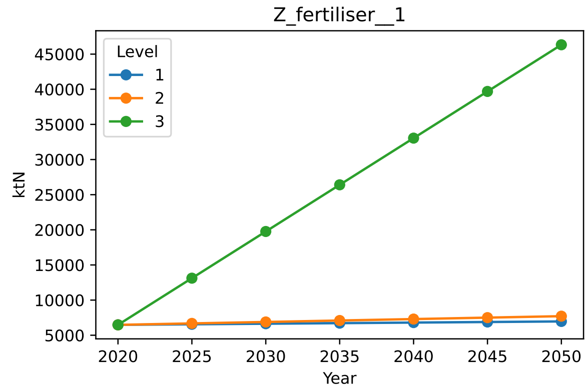
The regional total demand for synthetic nitrogen fertilizers in the demand reduction and fertiliser substitution scenario is the same as the demand reduction scenario, while the fractions are different. To gradually get rid of high-emitting nitrogen fertilisers, the fractions of urea, urea ammonium nitrate (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).

3.1 Parameter data

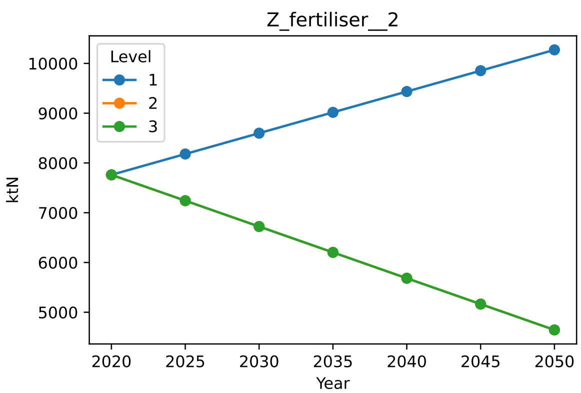
The plots below show the value over time of each parameter affected by this lever.



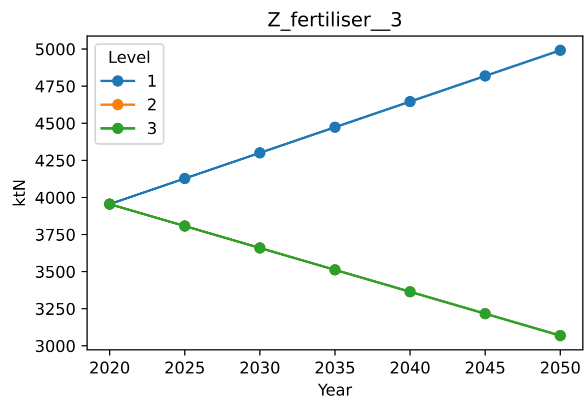
(a) Production of AmmoniaFertiliser



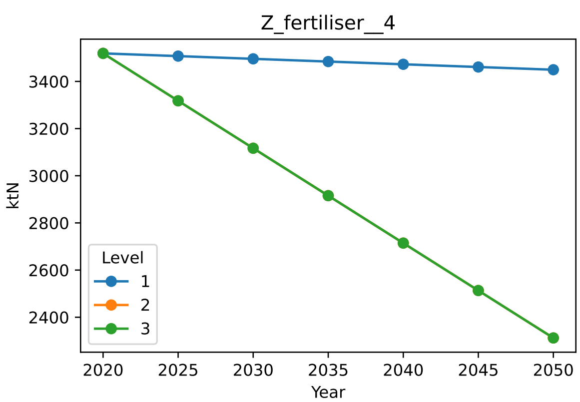
(b) Production of AmmoniumSulphate



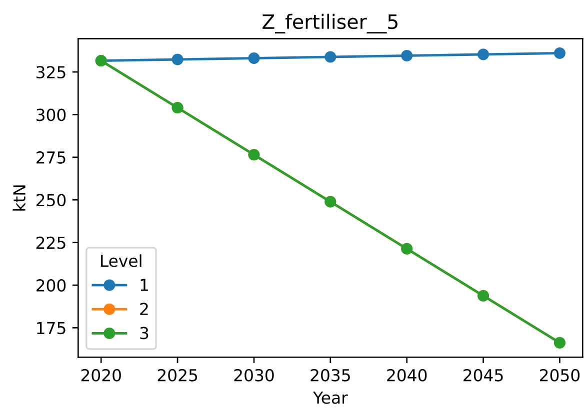
(c) Production of AmmoniumNitrate



(d) Production of CalciumAmmoniumNitrate

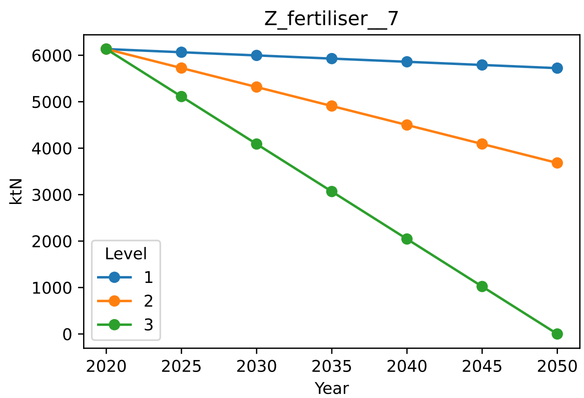


(e) Production of AmmoniumPhosphate

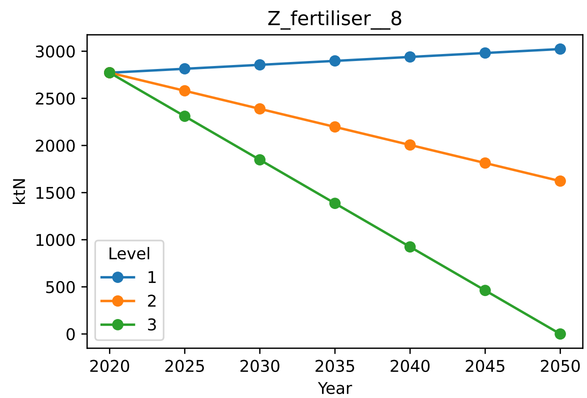


(f) Production of NKCompound

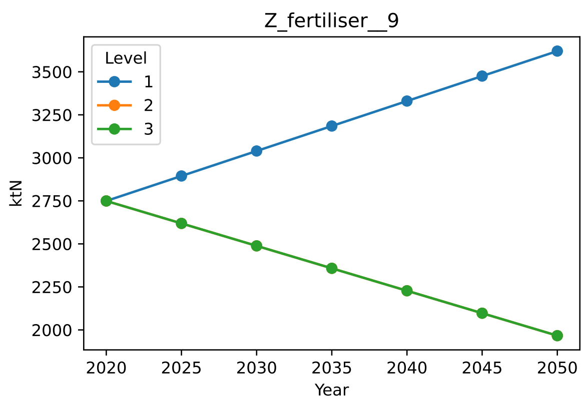
Figure 3.1: `fertiliser_demand` parameter data (part 1)



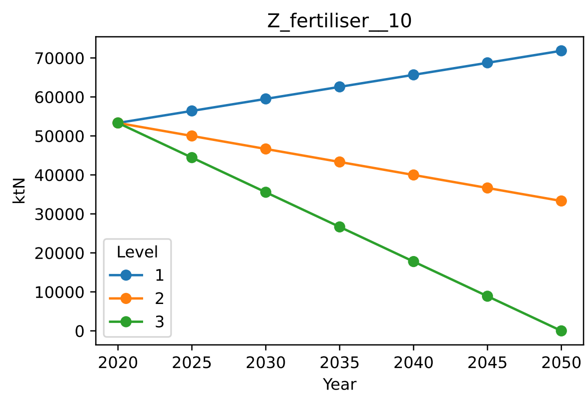
(a) Production of NPKCompound



(b) Production of UreaAmmoniumNitrate



(c) Production of OtherFertiliserN



(d) Production of OtherFertiliserNP

Figure 3.2: `fertiliser_demand` parameter data (part 2)

4 fertiliser_production

Lever ID fertiliser_production
Description Fertiliser production changes
Levels

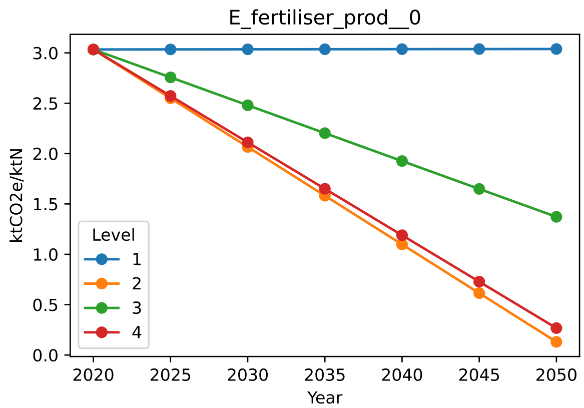
- *Level 1:* BAU
- *Level 2:* Water electrolysis
- *Level 3:* Electrical heating
- *Level 4:* CCS

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

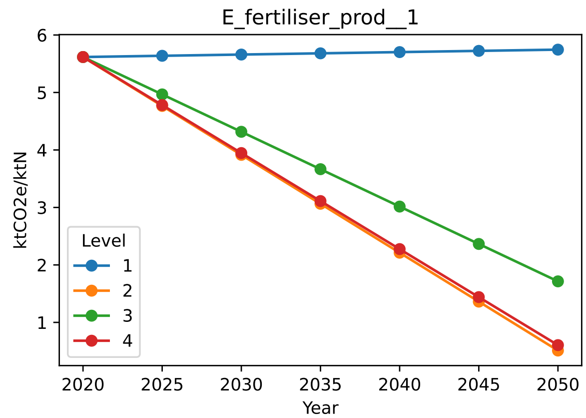
The production emission factors of various nitrogen fertilisers are constant in the BAU scenario. The production emission factors of each nitrogen fertiliser in water electrolysis, electrical heating and CCS scenarios in 2050 are estimated in our previous study (Gao and Cabrera Serrenho 2023). Note that 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.

4.1 Parameter data

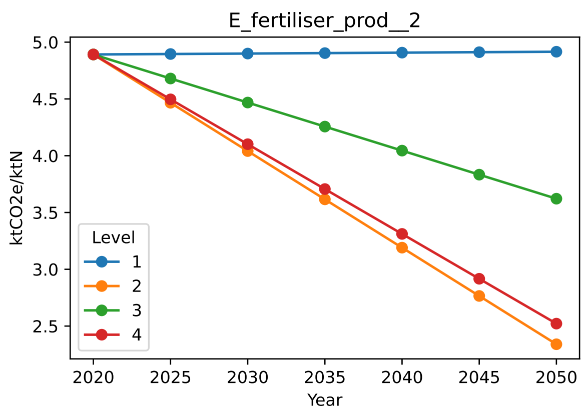
The plots below show the value over time of each parameter affected by this lever.



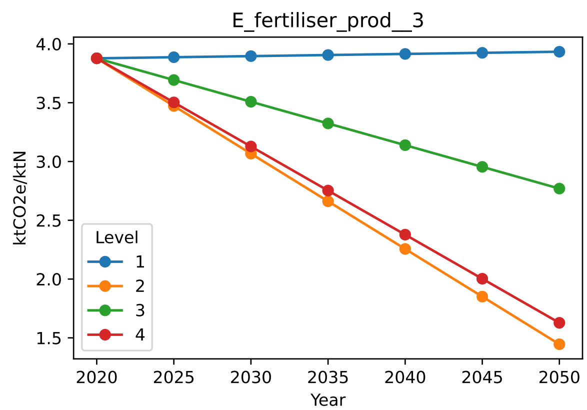
(a) Production of AmmoniaFertiliser



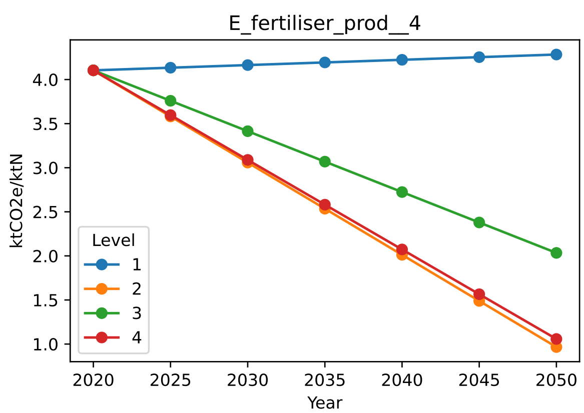
(b) Production of AmmoniumSulphate



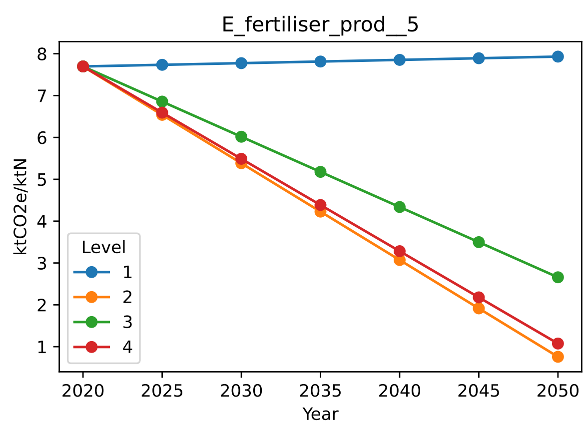
(c) Production of AmmoniumNitrate



(d) Production of CalciumAmmoniumNitrate

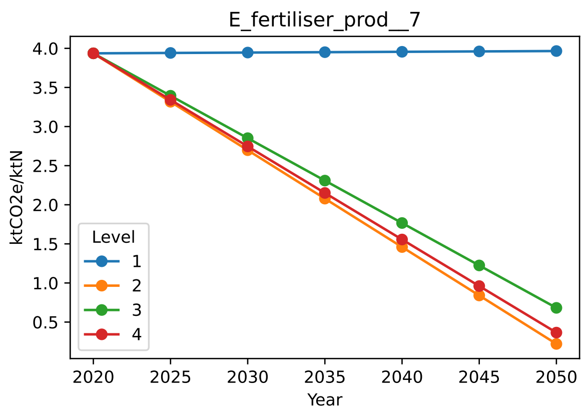


(e) Production of AmmoniumPhosphate

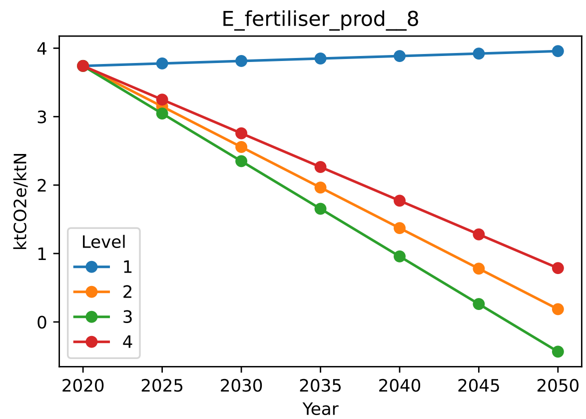


(f) Production of NKCompound

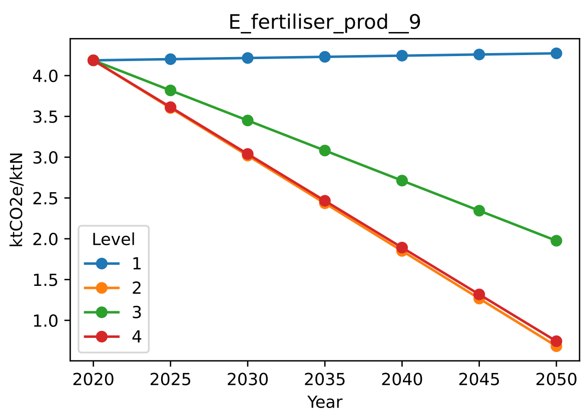
Figure 4.1: `fertiliser_production` parameter data (part 1)



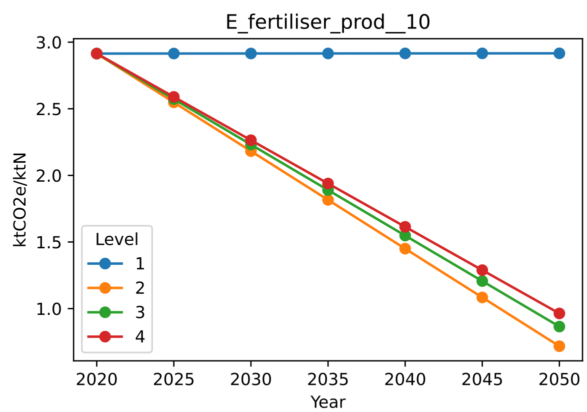
(a) Production of NPKCompound



(b) Production of UreaAmmoniumNitrate



(c) Production of OtherFertiliserN



(d) Production of OtherFertiliserNP

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

5 fertiliser_use_phase

Lever ID fertiliser_use_phase
Description Fertiliser use-phase changes
Levels

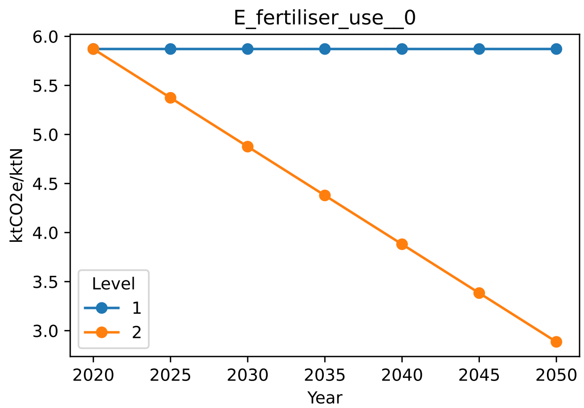
- *Level 1:* BAU
- *Level 2:* Nitrogen inhibitors

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

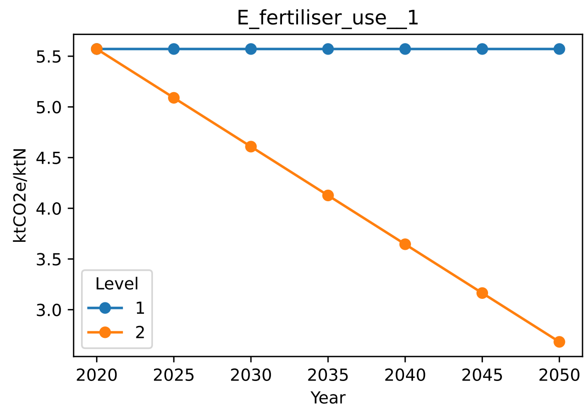
The use-phase emission factors of various nitrogen fertilisers are constant in the BAU scenario. In the nitrification inhibitor scenario, the use-phase emission factors in 2050 are calculated in our previous study (Gao and Cabrera Serrenho 2023). The use-phase emission factors are linearly interpolated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

5.1 Parameter data

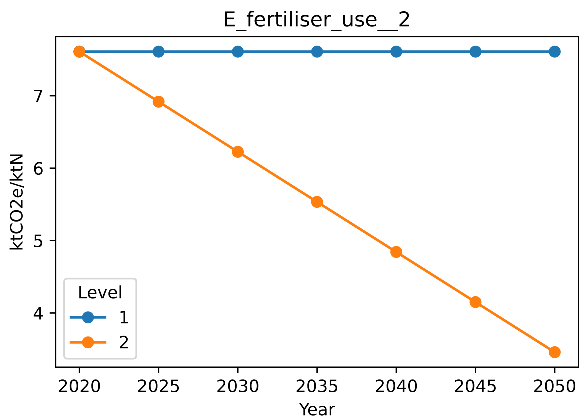
The plots below show the value over time of each parameter affected by this lever.



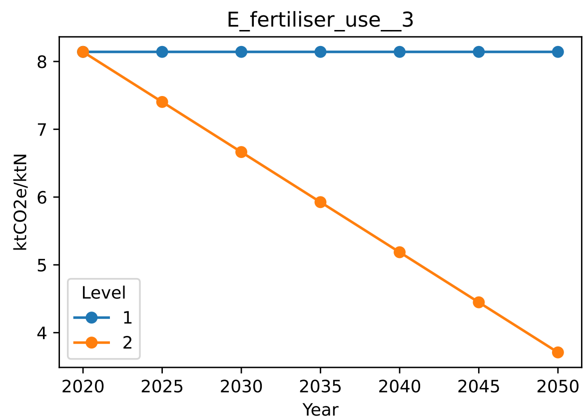
(a) Use of AmmoniaFertiliser



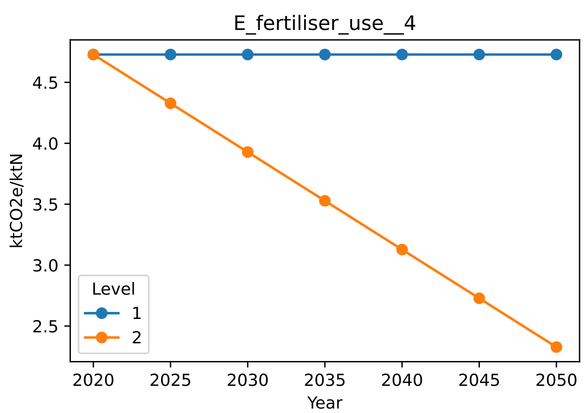
(b) Use of AmmoniumSulphate



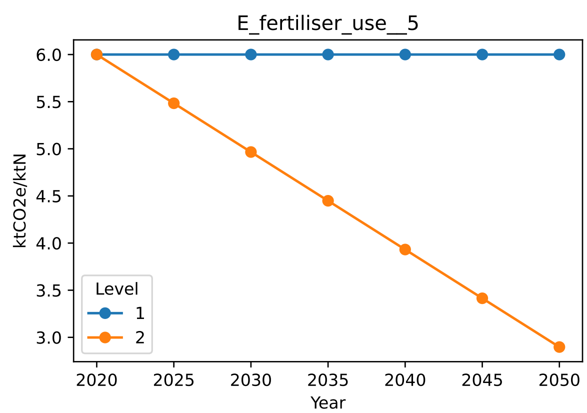
(c) Use of AmmoniumNitrate



(d) Use of CalciumAmmoniumNitrate

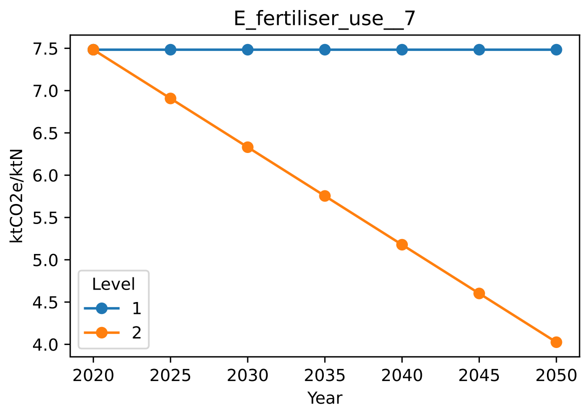


(e) Use of AmmoniumPhosphate

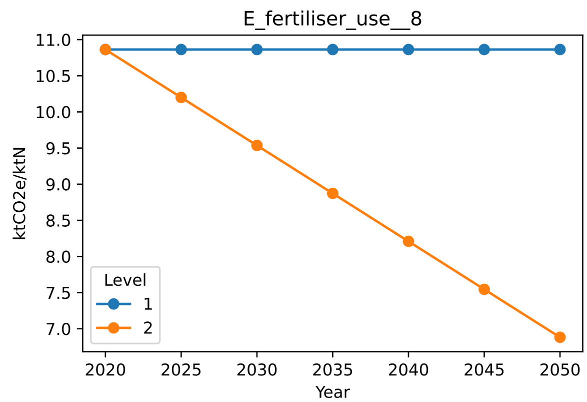


(f) Use of NKCompound

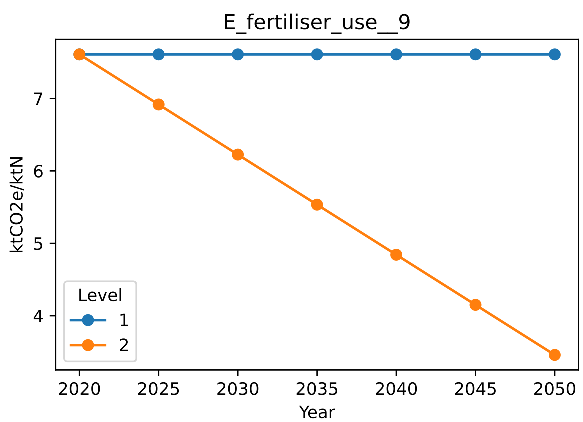
Figure 5.1: `fertiliser_use_phase` parameter data (part 1)



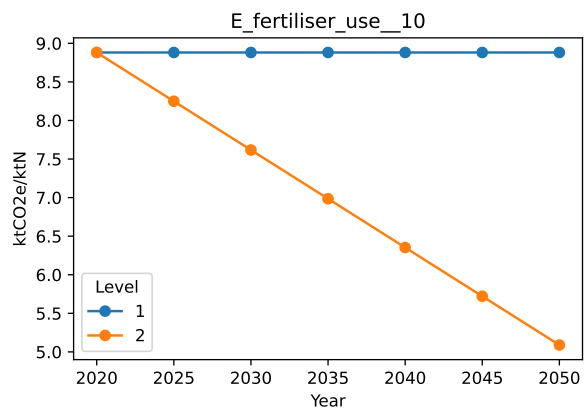
(a) Use of NPKCompound



(b) Use of UreaAmmoniumNitrate



(c) Use of OtherFertiliserN



(d) Use of OtherFertiliserNP

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

Part II

Demand model levers

6 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 a separate study by (**gao_evaluating_2024?**).

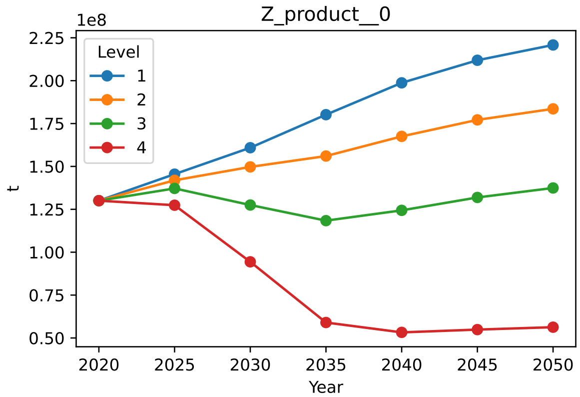
This uses a Dynamic Material Flow Analysis approach based on the assumption that, for durable goods, the per-capita stock of material in use is the more fundamental driver of material demand and waste flows. In the BAU scenario, the historical regional per-capita stock in each sector is correlated with 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_evaluating_2024?**).

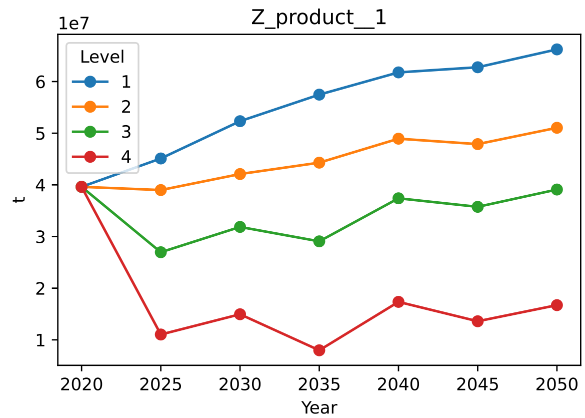
Similarly, for short-lived products such as packaging, the forecasted per-capita input increases as the fitted historical trend and forecasted GDP and population growth in the BAU scenario. In demand reduction scenarios, the regional input flow per capita is assumed to be capped to certain percentages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

6.1 Parameter data

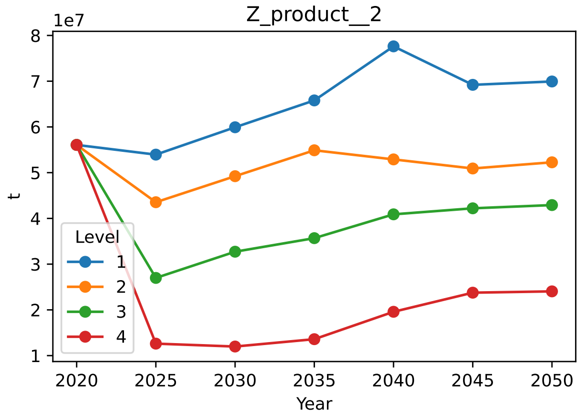
The plots below show the value over time of each parameter affected by this lever.



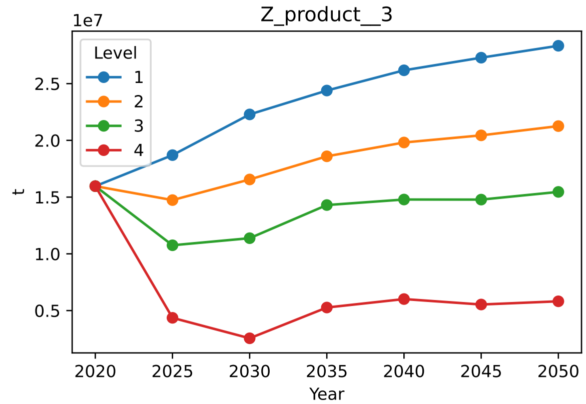
(a) Demand for Packaging



(b) Demand for Transportation

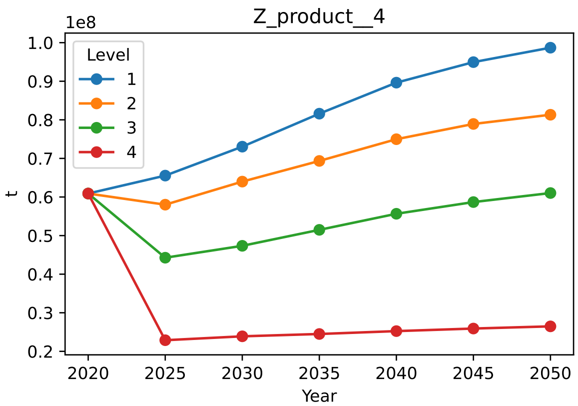


(c) Demand for BuildingsAndConstruction

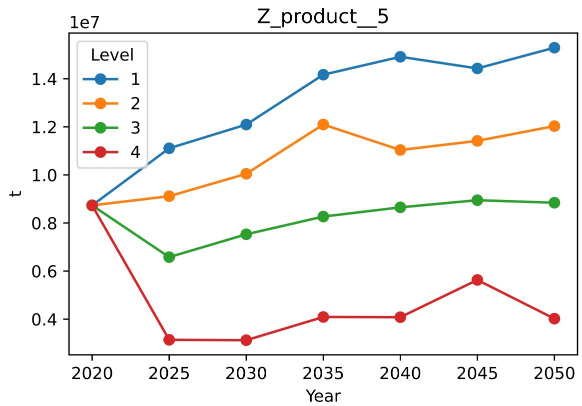


(d) Demand for ElectricalAndElectronic

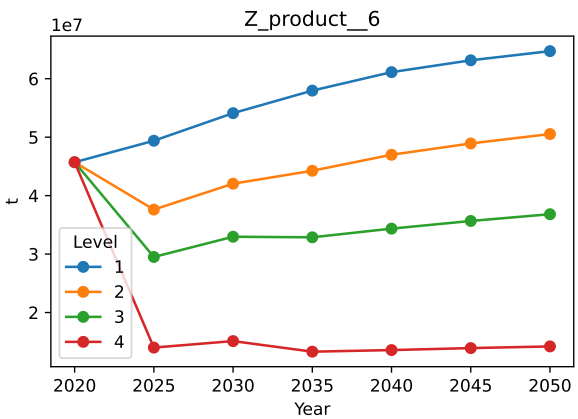
Figure 6.1: `product_demand` parameter data (part 1)



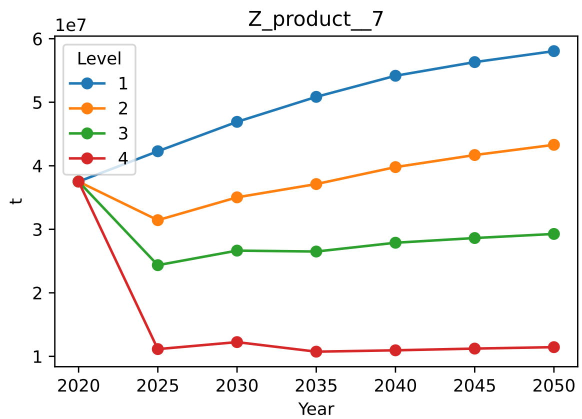
(a) Demand for ConsumerAndInstitutional



(b) Demand for IndustrialMachinery

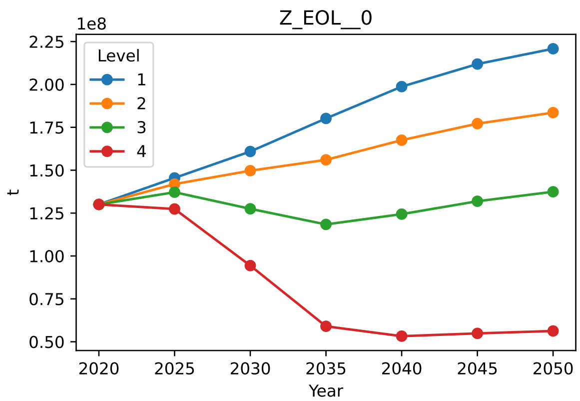


(c) Demand for Textile

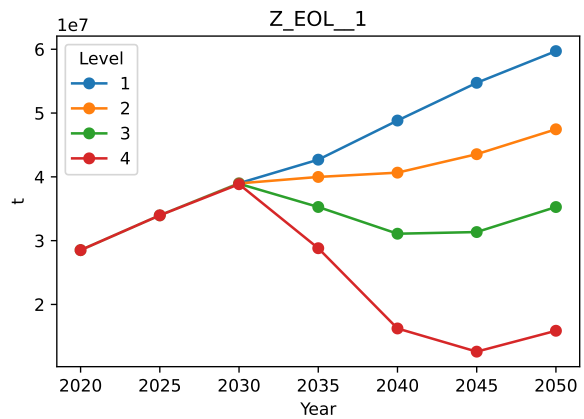


(d) Demand for Other

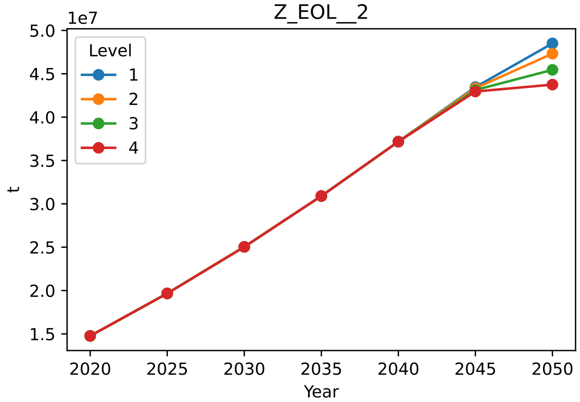
Figure 6.2: `product_demand` parameter data (part 2)



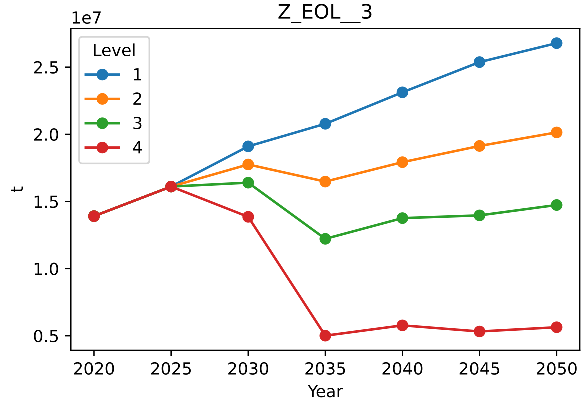
(a) EOL from Packaging



(b) EOL from Transportation

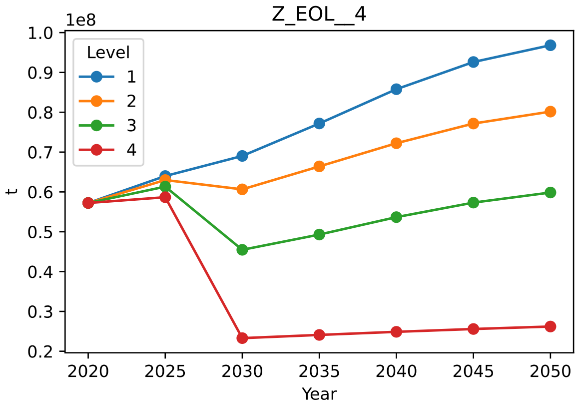


(c) EOL from BuildingsAndConstruction

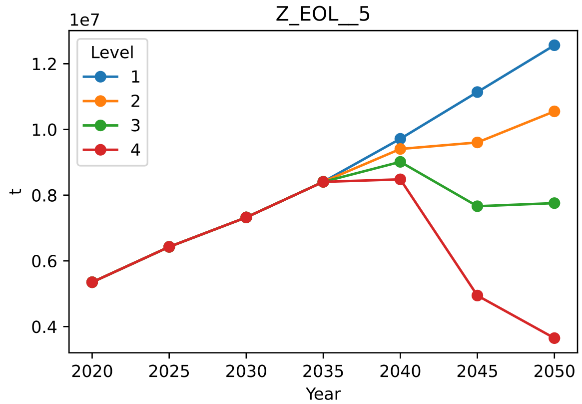


(d) EOL from ElectricalAndElectronic

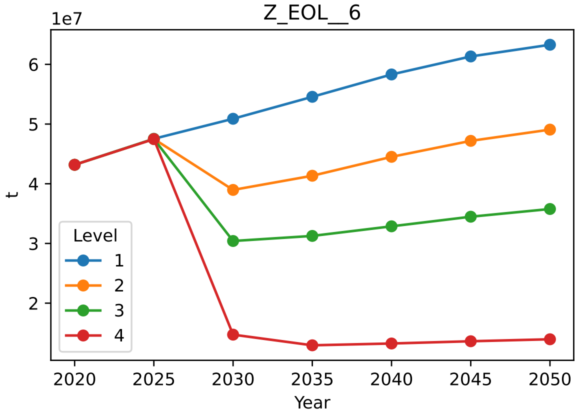
Figure 6.3: `product_demand` parameter data (part 3)



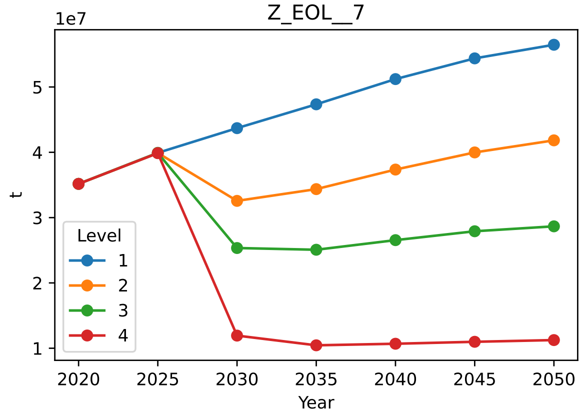
(a) EOL from ConsumerAndInstitutional



(b) EOL from IndustrialMachinery



(c) EOL from Textile



(d) EOL from Other

Figure 6.4: `product_demand` parameter data (part 4)

7 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 HDPE, LDPE, LLDPE, PP, PS, PET, PVC, and Fibre PPA. They can be melted and formed again to original state with little to no loss in properties. It makes sense to mechanically recycle them.

- Thermosets involve crosslinking such as PUR and Styrene-Butadiene Rubber. Other polymers were placed under this category for simplicity. Melting them tend to induce curing and can change their properties. It does not make sense to mechanical recycle them. There is in literature mentioning cutting them up and re-using them, which is not mechanical recycling in the sense we want them back to their original form and purpose. Hence, chemical recycling that break down to their feedstock and/or monomer makes sense as these can be used to produce the original polymer back.

7.1 Possible recycling routes

First the possible recycling routes in different scenarios are set for 3 levels of ambition, as summarised in Table 7.1.

Table 7.1: 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
Synthetic rubber	_ / _	_ / _	_ / C
Other polymers	_ / _	_ / _	_ / C

7.1.1 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 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, 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, it there is limited recycling, with most going to incineration and land filling (Hirschberg and Rodrigue 2023).

7.1.2 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 Lewandowski and Skórczewska (2022).
- PS and PET can be both mechanically and chemically recycled.
- Mechanical recycling degrades the polymer properties of thermosettting PURs (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.

7.2 Quantifying recycling rates

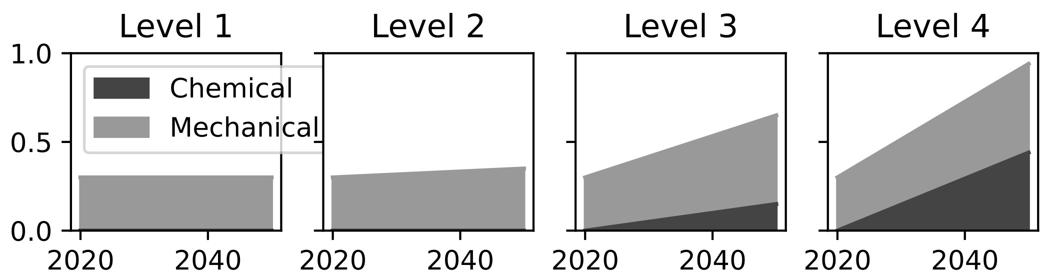
The baseline overall global recycling rate is 9% according to OECD (2022). This is distributed across the relevant polymers for each level Table 7.1 based on the mass flow quantities of each polymer in the baseline model. The recycling rate for PP is 1% (Basham 2019), and equal recycling rates for HDPE, 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 7.1 at 15% for LLDPE and 5% for others.

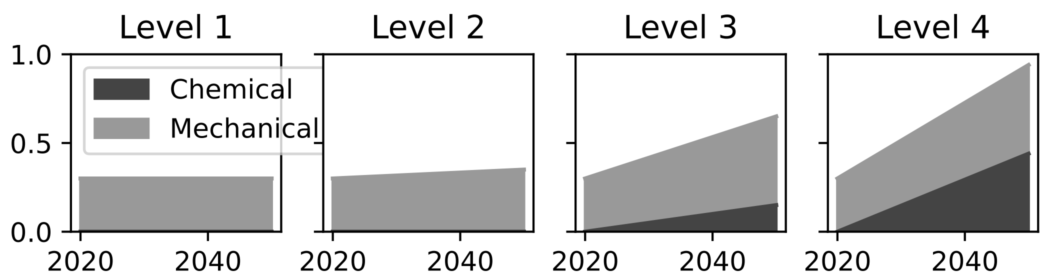
The more ambitious scenario from OECD (2022) reaches 47% overall recycling rate by 2050. This increase is achieved by increasing recycling rates to 50% for all polymers which can be mechanically recycled in Table 7.1, together with 15% chemical recycling of all polymers.

7.3 Parameter data

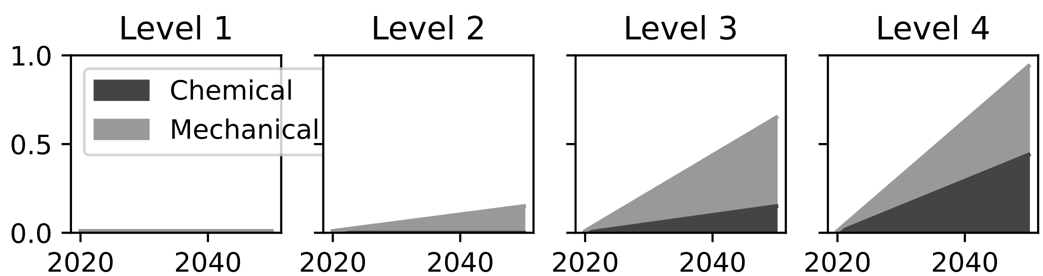
The plots below show the change in recycling rates over time for each polymer affected by this lever.



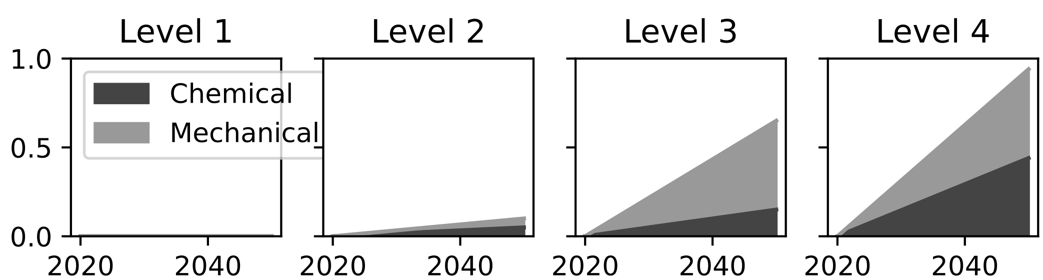
(a) LDPEPolyethylene



(b) HDPEPolyethylene

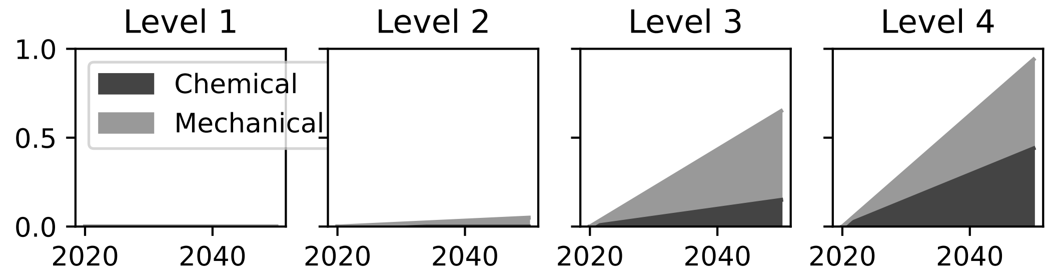


(c) PPPolypropylene

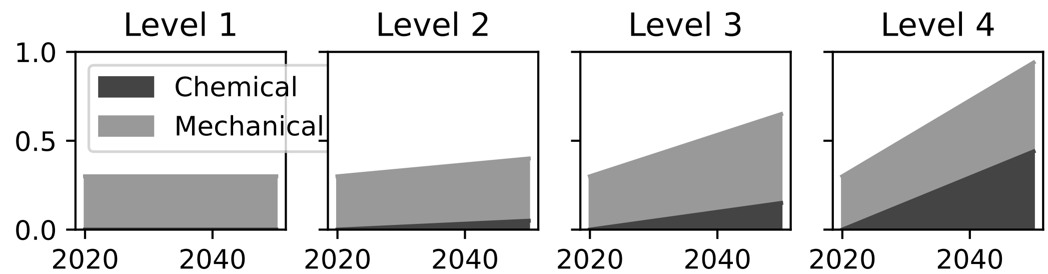


(d) PSPolystyrene

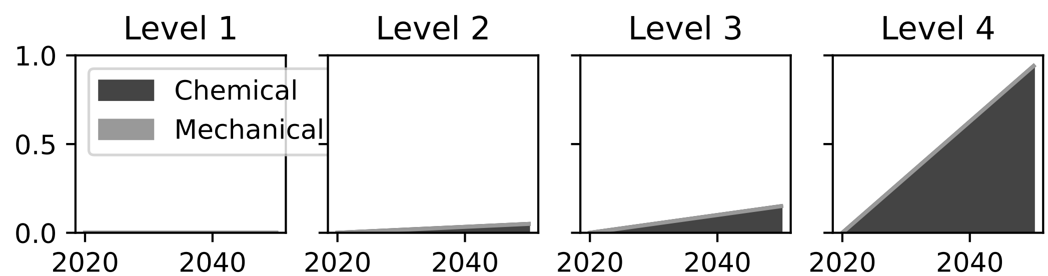
Figure 7.1: `recycling` parameter data (part 1)



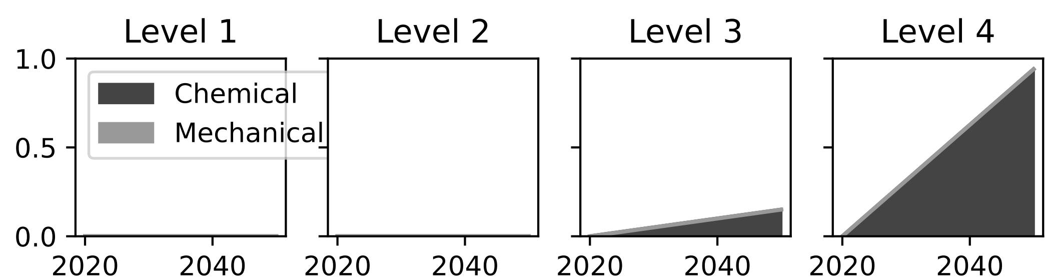
(a) PVCPolyvinylChloride



(b) PETPolyethyleneTerephthalatePolyesters

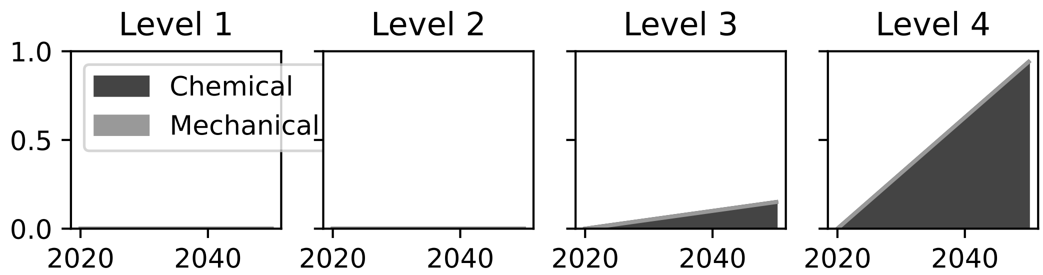


(c) Polyurethane

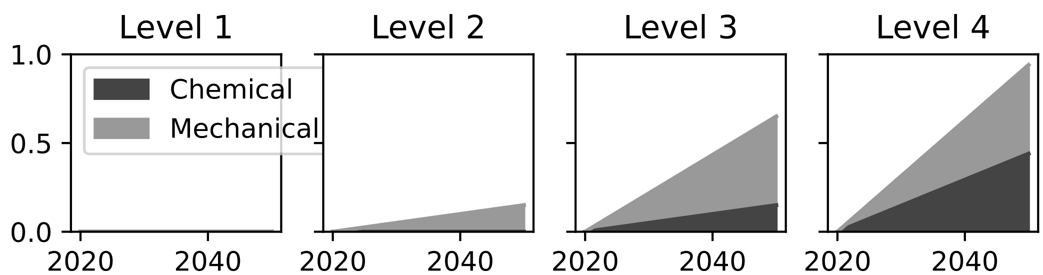


(d) SyntheticRubbers

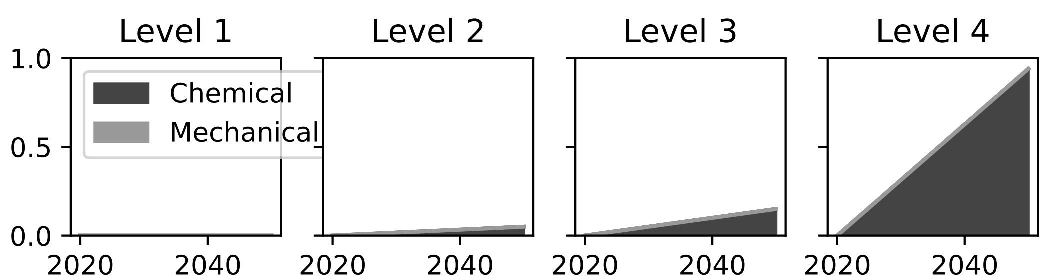
Figure 7.2: `recycling` parameter data (part 2)



(a) OtherPolymers



(b) LLDPE



(c) FibrePPA

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

8 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

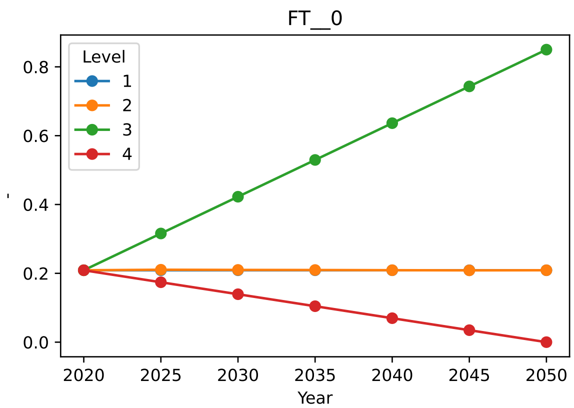
This lever controls how much non-recycled end-of-life material is sent to different destinations.

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

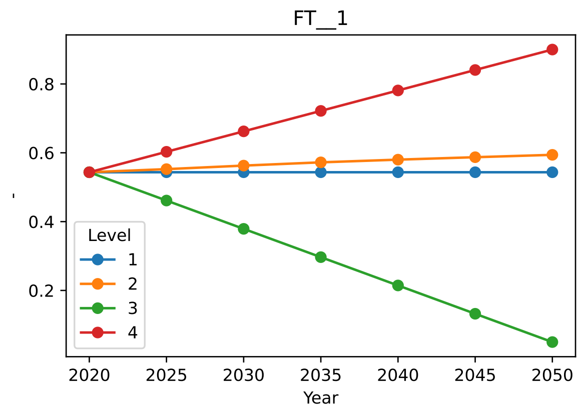
To consider different possible end-of-life options which effect GHG emissions, additional lever levels are added with very high incineration and landfilling shares respectively. A residual 10% share for mismanagement is assumed to persist.

8.1 Parameter data

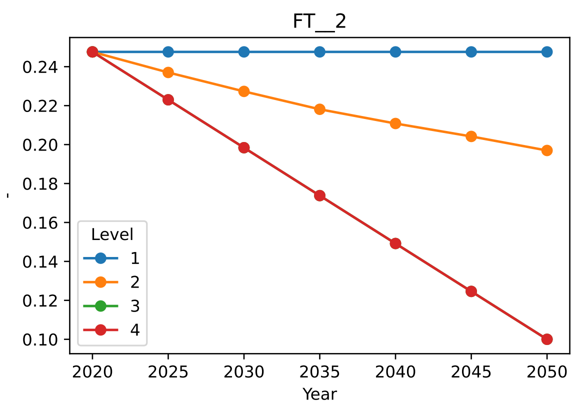
The plots below show the value over time of each parameter affected by this lever.



(a) Incineration



(b) Landfilling



(c) Mismanagement

Figure 8.1: `final_treatment` parameter data

9 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).

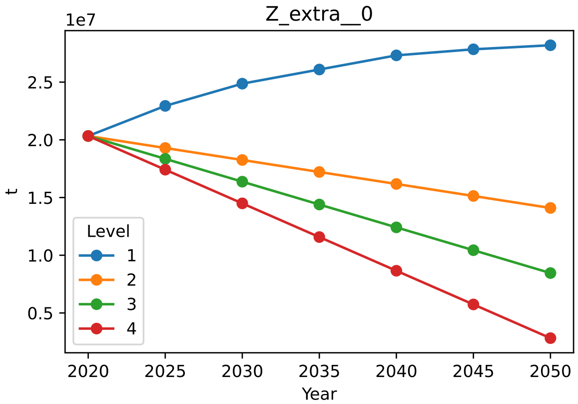
The baseline level of extra demand has been calibrated based on total global demand for BTX and methyl alcohol (**icis_supply_XXX?**), .

The reference projection is based on projected growth in demand for BTX (**icis_supply_XXX?**), 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 Institute (2023).

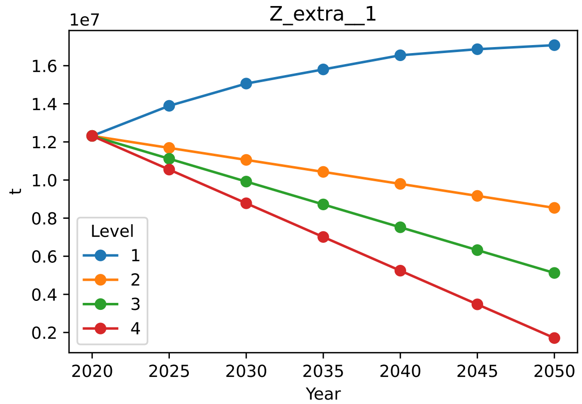
The demand-reduction scenarios then scale down from this projected demand proportionally, to illustrate how different supply-side scenarios are affected by changes in demand levels.

9.1 Parameter data

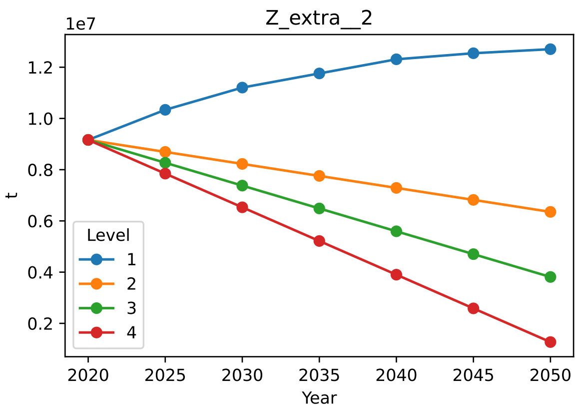
The plots below show the value over time of each parameter affected by this lever.



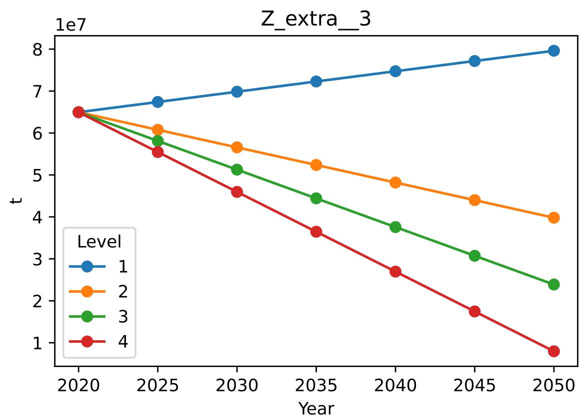
(a) Benzene



(b) Toluene



(c) Xylenes



(d) MethylAlcohol

Figure 9.1: `extra_demand` parameter data

Part III

Petrochemical production levers

10 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

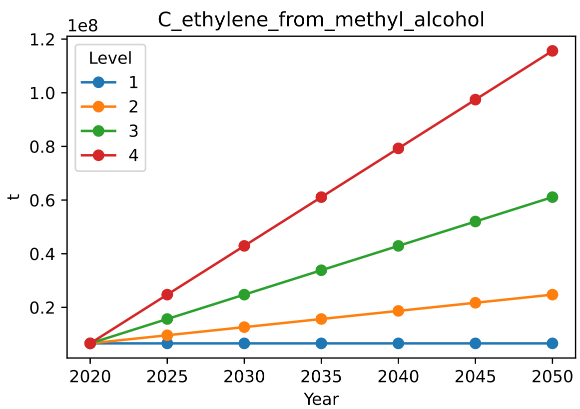
This lever controls the available capacity of MTO (Methanol-to-Olefins), measured by the ethylene production capacity.

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 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.

10.1 Parameter data



11 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

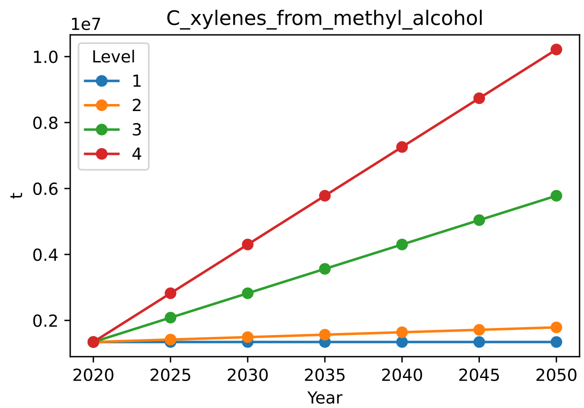
This lever controls the available capacity for producing BTX from methyl alcohol ("Methanol-to-aromatics", or MTA), measured by the Xylene production capacity.

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

Capacities are estimated based on data from Pales et al. (2018b), who report projections for MTA and MTO (methanol-to-olefins) together. They report capacity will peak by 2030 and then decline, due to decline in coal-based methanol after 2030. However, we assume MTO/MTA will continue due to the emergence of renewable methanol, which is expected to be cost-competitive by 2050 given the right policies (**irena_innovation_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 10), we obtained the MTA growth. The values are comparable in magnitude to the existing size of the MTA demonstration plants reported by (**wang_methanol_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


C_xylenes_from_methyl_alcohol
1e7
Level
1
2
3
4
1.0
0.8
0.6
0.4
0.2
t
2020
2025
2030
2035
2040
2045
2050
Year

12 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

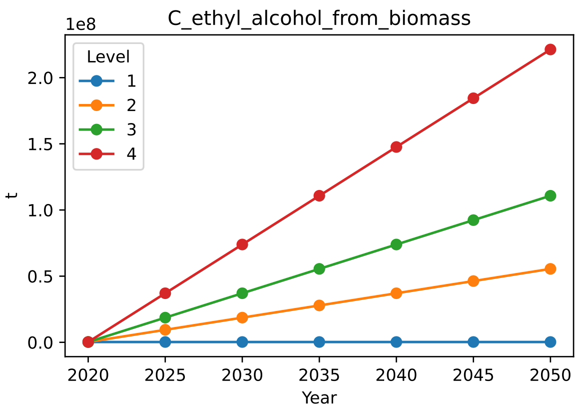
This lever controls the available capacity for producing ethylene from bio-ethyl-alcohol, measured by the ethyl alcohol production capacity.

Baseline total bioethanol production is reported by (**opec_world_2022?**) and agrees well with (**doe_global_2022?**) (3% difference). Of this, the majority is used as fuel, with 0.3% used for ethylene production (**mohsenzadeh_bioethylene_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 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_world_2022?**).

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

12.1 Parameter data


C_ethyl_alcohol_from_biomass
1e8
Level
1
2
3
4
t
0.0
0.5
1.0
1.5
2.0
2020
2025
2030
2035
2040
2045
2050
Year

13 biosyngas_capacity

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

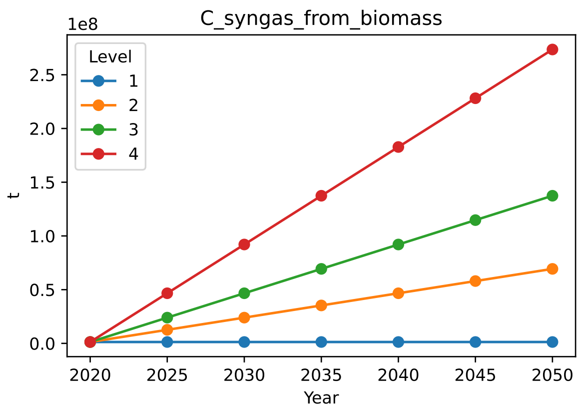
- *Level 1:* Baseline capacity
- *Level 2:* 50% of projected growth in biomass for bioethanol used for syngas
- *Level 3:* 100% of projected growth in biomass for bioethanol used for syngas
- *Level 4:* 200% of projected growth in biomass for bioethanol used for syngas

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

Based on figures from (**barton_gstc_2021?**), global capacity for syngas production from biomass is about 1.3 Mt/year, with 94 Mt/year from "other" sources which is assumed to be wastes that are 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_innovation_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 downstream uses. 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 12), adjusting for the significantly higher yield of syngas than ethanol per unit mass of biomass.

13.1 Parameter data


C_syngas_from_biomass
1e8
Level
1
2
3
4
2.5
2.0
1.5
1.0
0.5
0.0
t
2020
2025
2030
2035
2040
2045
2050
Year

14 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). Accounting for the ethanol yield from each biomass feedstock gives a baseline share of 72% ethanol from maize, 28% from sugarcane.

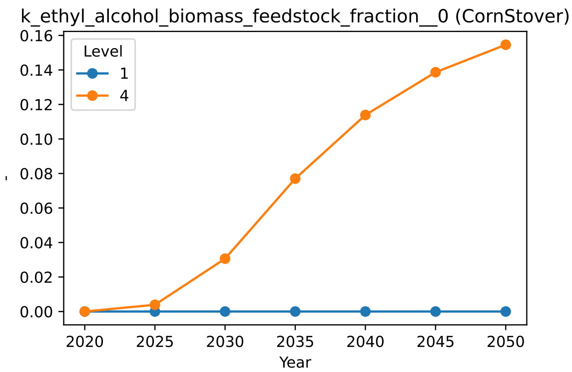
Historical global production of sugar cane, maize, [paddy] rice, and wheat were obtained from FAO (2024), and the trendline used to project production from 2020 to 2050. Using typical sugarcane bagasse to sugarcane ratio by Nikodinovic-Runic et al. (2013), corn stover to maize ratio by Ruan et al. (2019), rice straw to paddy rice ratio (IRRI 2018), and wheat straw to wheat ratio by Song et al. (2013), corresponding production of these residues can also be estimated.

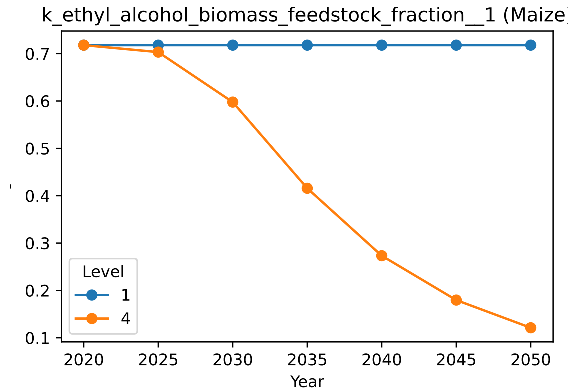
The fraction of the biomass available for ethanol production is 26% of the total sugar cane production and 14% of the total maize production using the data from (FAO 2024), (Gro Intelligence 2019), and (USDA 2023). Similar to the work of Meng et al. (2023), 20% of the total crop residues produced are assumed to be available for chemical production.

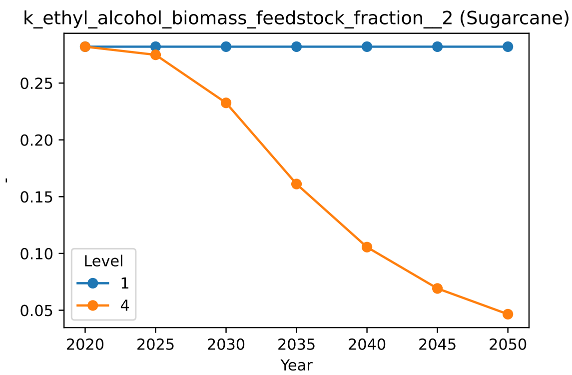
In future the balance of ethanol from edible sugars vs lignocellulosic biomass is expected to shift. Lash et al (2022) projected the future contributions of these to total fuel from 2020 to 2050, which is assumed to also apply to ethanol for chemicals. Together, after adjusting for ethanol yields, these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

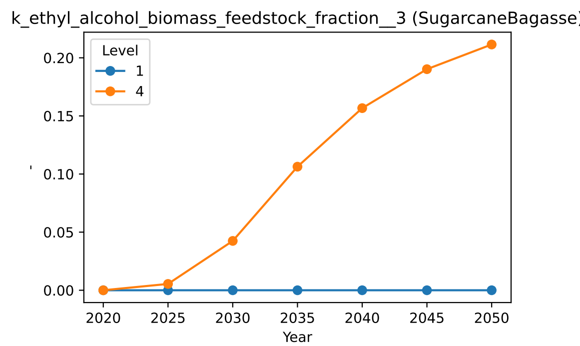
Feedstock shares used for biosyngas are assumed to be the same as for the lignocellulosic biomass used for bioethanol.

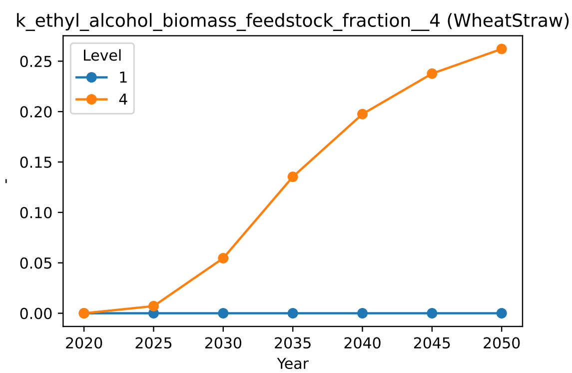
14.1 Parameter data

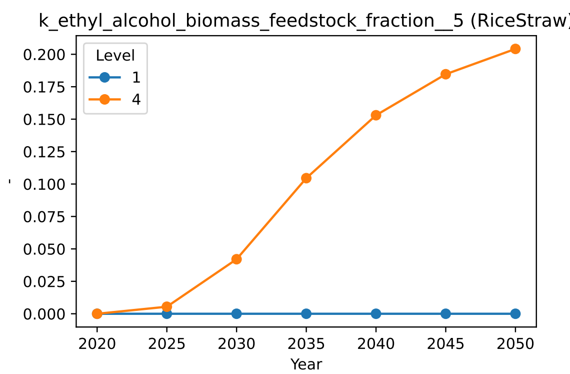

k_ethyl_alcohol_biomass_feedstock_fraction__0 (CornStover)
Level
1
4
Year

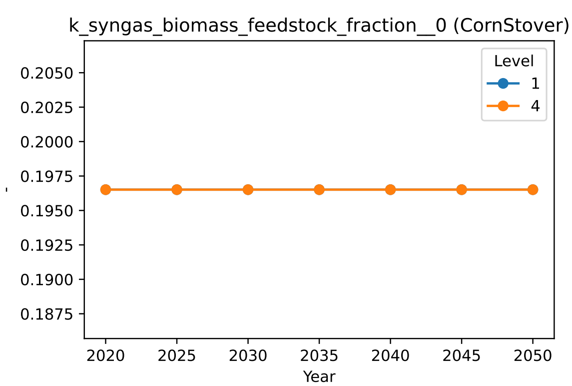

k_ethyl_alcohol_biomass_feedstock_fraction__1 (Maize)
Level
1
4
Year

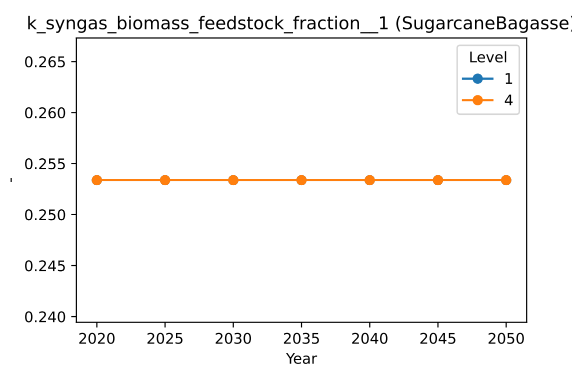

k_ethyl_alcohol_biomass_feedstock_fraction__2 (Sugarcane)
Level
1
4
Year

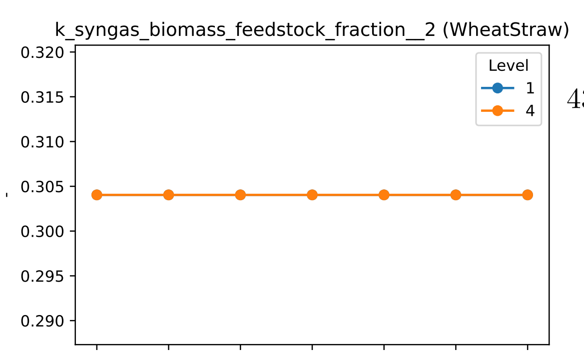

k_ethyl_alcohol_biomass_feedstock_fraction__3 (SugarcaneBagasse)
Level
1
4
Year

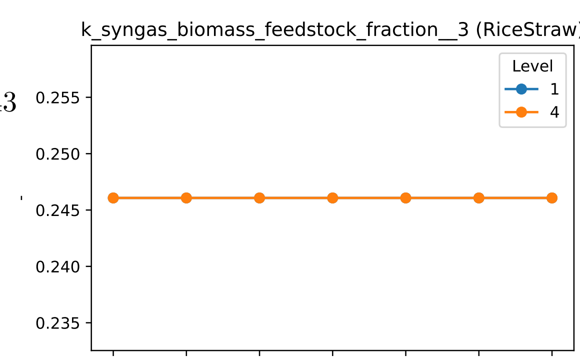

k_ethyl_alcohol_biomass_feedstock_fraction__4 (WheatStraw)
Level
1
4
Year


k_ethyl_alcohol_biomass_feedstock_fraction__5 (RiceStraw)
Level
1
4
Year


k_syngas_biomass_feedstock_fraction__0 (CornStover)
Level
1
4
Year


k_syngas_biomass_feedstock_fraction__1 (SugarcaneBagasse)
Level
1
4
Year


k_syngas_biomass_feedstock_fraction__2 (WheatStraw)
Level
1
4


k_syngas_biomass_feedstock_fraction__3 (RiceStraw)
Level
1
4

15 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

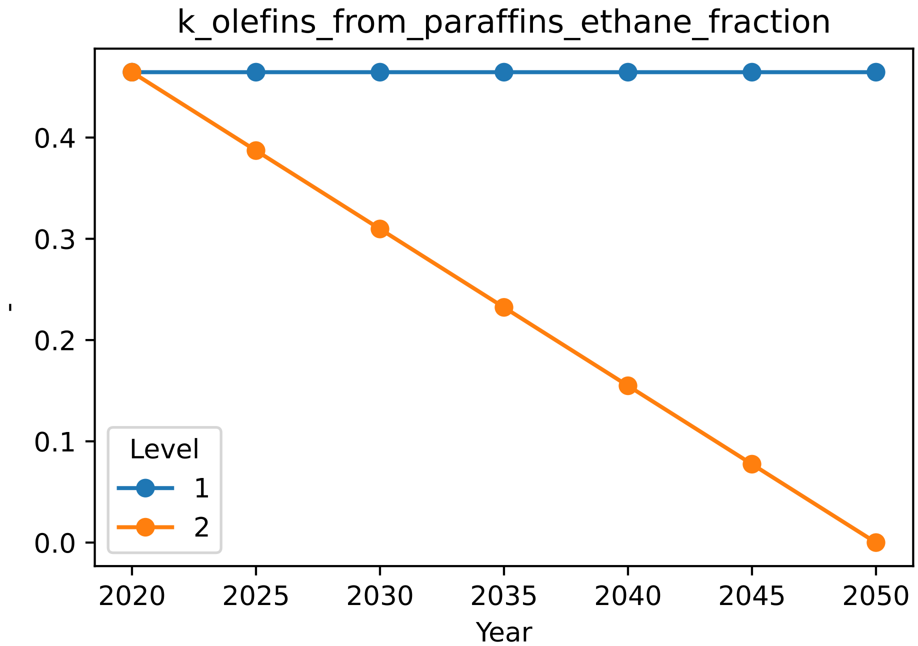
- *Level 1:* Baseline fraction of ethane
- *Level 2:* Replace ethane use with naphtha

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_supply_XXX?**). 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.

15.1 Parameter data



Part IV

Hydrogen levers

16 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.

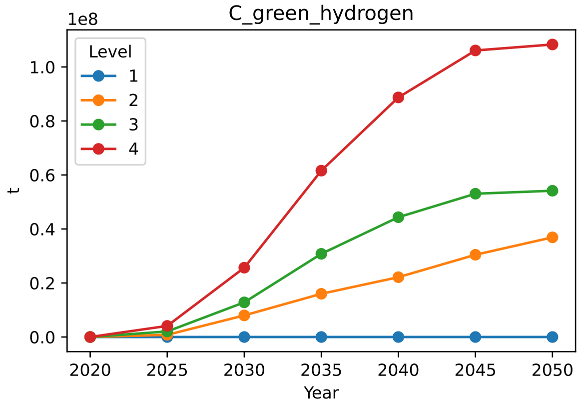
Currently this route is not used, so the baseline capacity remains at zero.

Growth scenarios are based on the Hydrogen Council and McKinsey & Company (2023) Hydrogen Outlook. They project 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.

16.1 Parameter data


C_green_hydrogen
1e8
Level
1
2
3
4
1.0
0.8
0.6
0.4
0.2
0.0
t
2020
2025
2030
2035
2040
2045
2050
Year

17 blue_hydrogen_capacity

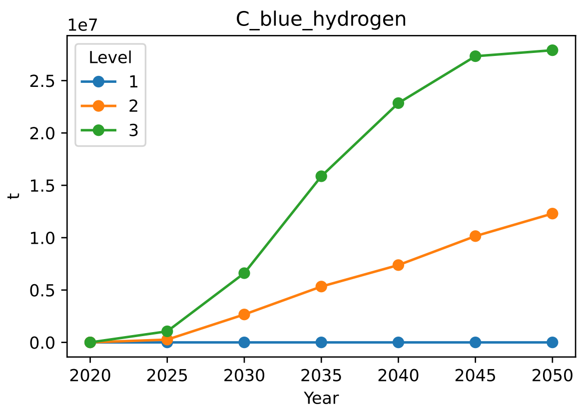
Lever ID blue_hydrogen_capacity
Description Sets the total capacity to produce "blue" hydrogen via natural gas steam methane reforming with CCS
Levels

- *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 CCS (carbon capture and storage).

The values were derived as described in Chapter 16.

17.1 Parameter data



Part V

Abatement levers

18 ccs_incineration

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

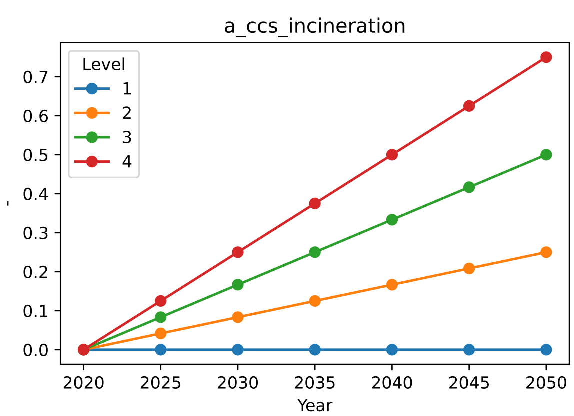
- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

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

Currently practically no Carbon Capture and Storage (CCS) is in use, 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.

18.1 Parameter data



19 ccs_process_emissions

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

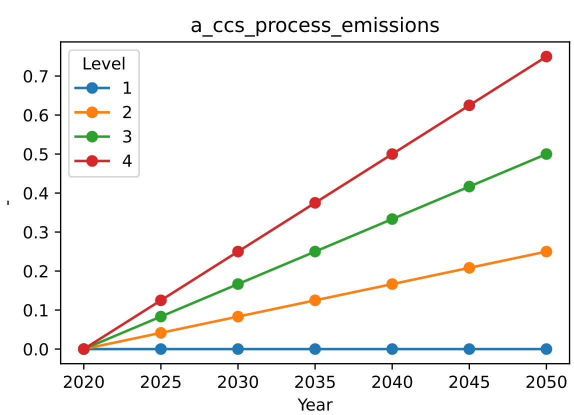
- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

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

Currently practically no Carbon Capture and Storage (CCS) is in use, 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.

19.1 Parameter data



20 ccs_utility_combustion

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

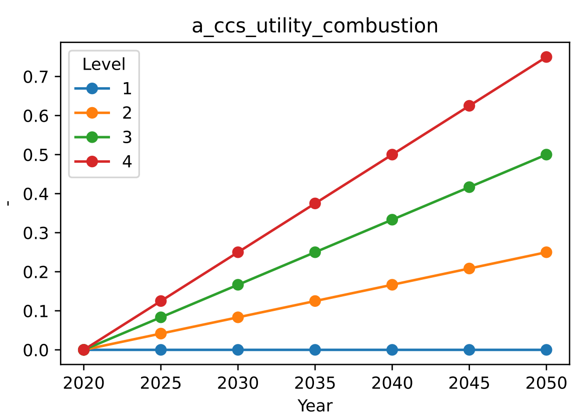
- *Level 1:* No abatement
- *Level 2:* 25% abatement
- *Level 3:* 50% abatement
- *Level 4:* 75% abatement

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

Currently practically no Carbon Capture and Storage (CCS) is in use, 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.

20.1 Parameter data



Part VI

Utilities & emissions data

21 electricity_requirements

Lever ID electricity_requirements
Description
Levels

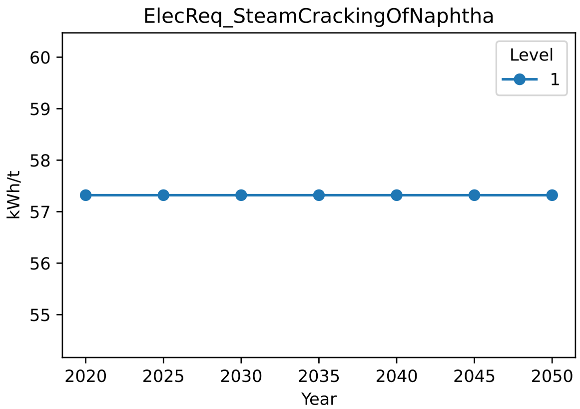
- *Level 1:* Baseline/constant

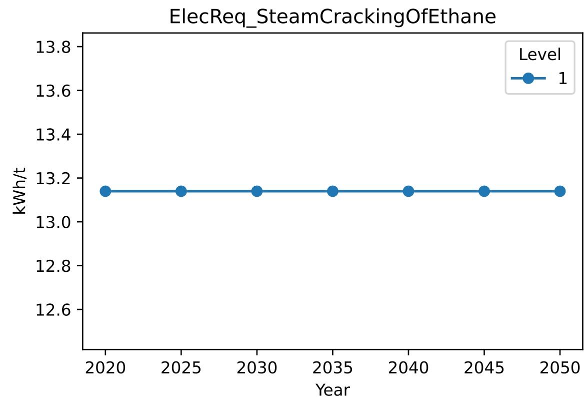
This lever sets the baseline values for electricity utility requirements for all processes.

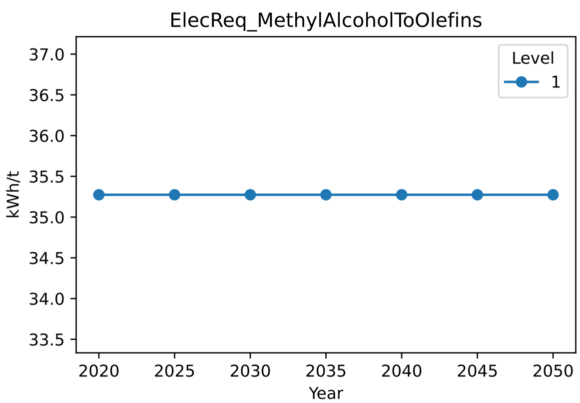
Data was sourced from Zhao et al. (2021), Jiang et al. (2020), Rosental et al. (2020), Oni et al. (2022), IEA (2021), and cross-checked against data from IHS (XXX) to estimate indicative electricity requirements for each process.

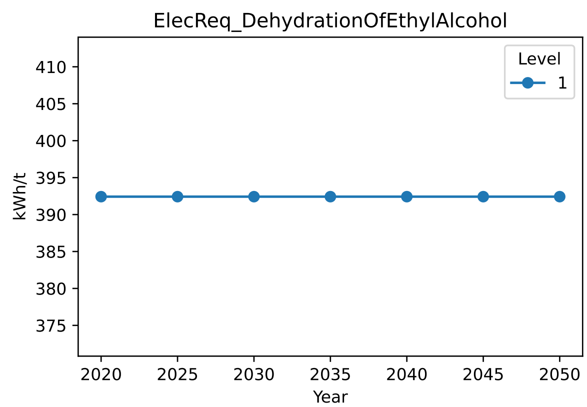
21.1 Parameter data

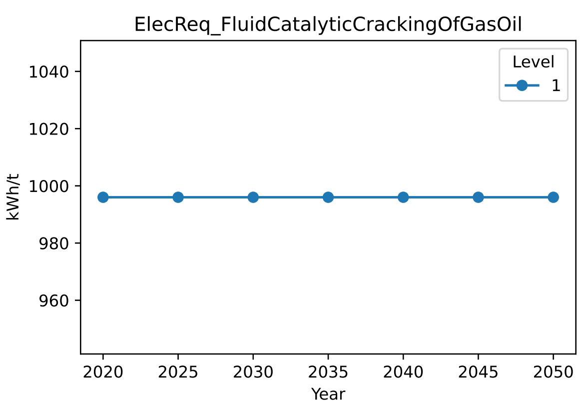
```
/opt/homebrew/Caskroom/miniconda/base/envs/cthru-calculator/lib/python3.10/site-packages/panc
  fig = self.plt.figure(figsize=self.figsize)
```

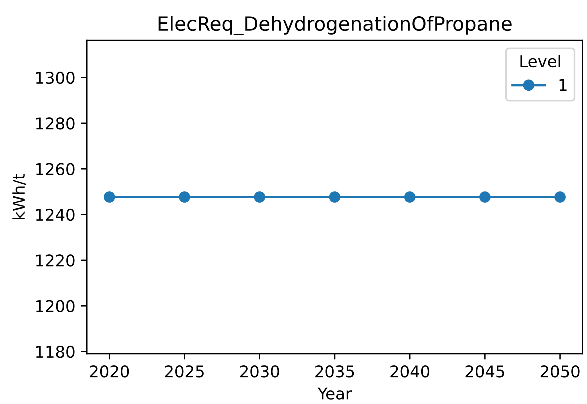

ElecReq_SteamCrackingOfNaphtha
Level
1
kWh/t
60
59
58
57
56
55
2020
2025
2030
2035
2040
2045
2050
Year

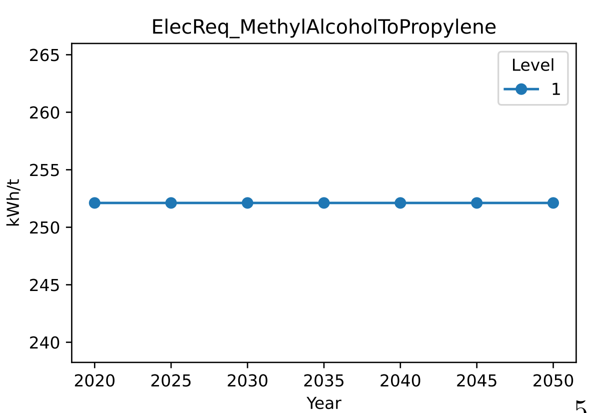

ElecReq_SteamCrackingOfEthane
Level
1
kWh/t
13.8
13.6
13.4
13.2
13.0
12.8
12.6
2020
2025
2030
2035
2040
2045
2050
Year

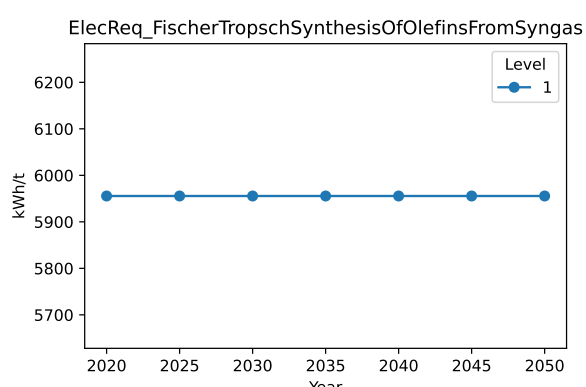

ElecReq_MethylAlcoholToOlefins
Level
1
kWh/t
37.0
36.5
36.0
35.5
35.0
34.5
34.0
33.5
2020
2025
2030
2035
2040
2045
2050
Year

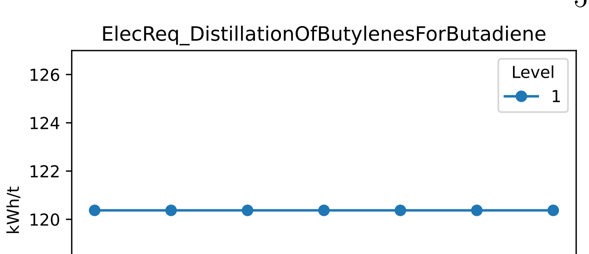

ElecReq_DehydrationOfEthylAlcohol
Level
1
kWh/t
410
405
400
395
390
385
380
375
2020
2025
2030
2035
2040
2045
2050
Year

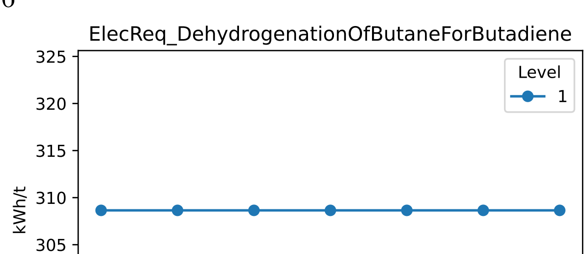

ElecReq_FluidCatalyticCrackingOfGasOil
Level
1
kWh/t
1040
1020
1000
980
960
2020
2025
2030
2035
2040
2045
2050
Year


ElecReq_DehydrogenationOfPropane
Level
1
kWh/t
1300
1280
1260
1240
1220
1200
1180
2020
2025
2030
2035
2040
2045
2050
Year


ElecReq_MethylAlcoholToPropylene
Level
1
kWh/t
265
260
255
250
245
240
2020
2025
2030
2035
2040
2045
2050
Year


ElecReq_FischerTropschSynthesisOfOlefinsFromSyngas
Level
1
kWh/t
6200
6100
6000
5900
5800
5700
2020
2025
2030
2035
2040
2045
2050
Year


ElecReq_DistillationOfButylenesForButadiene
Level
1
kWh/t
126
124
122
120


ElecReq_DehydrogenationOfButaneForButadiene
Level
1
kWh/t
325
320
315
310
305

22 natural_gas_requirements

Lever ID natural_gas_requirements
Description
Levels

- *Level 1:* Baseline/constant

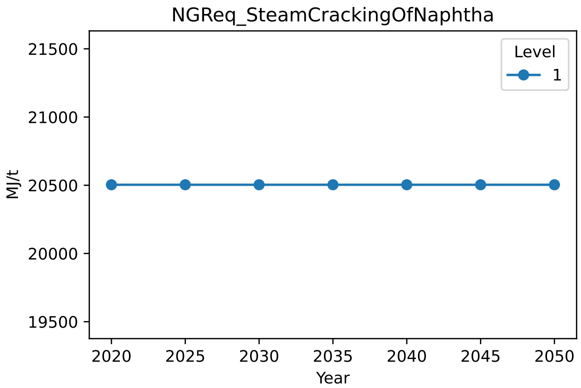
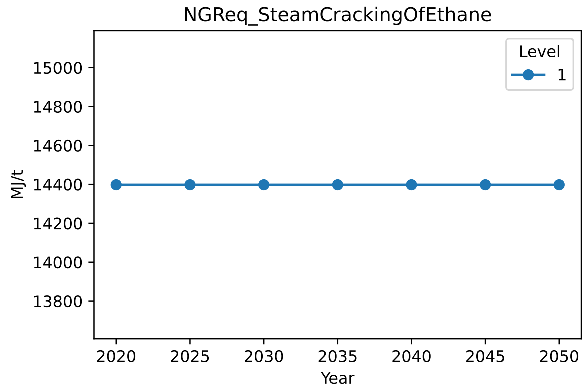
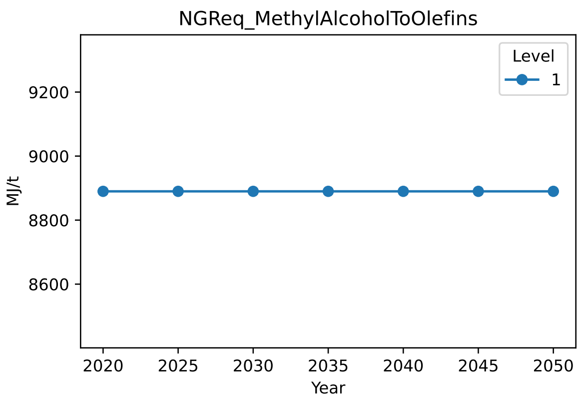
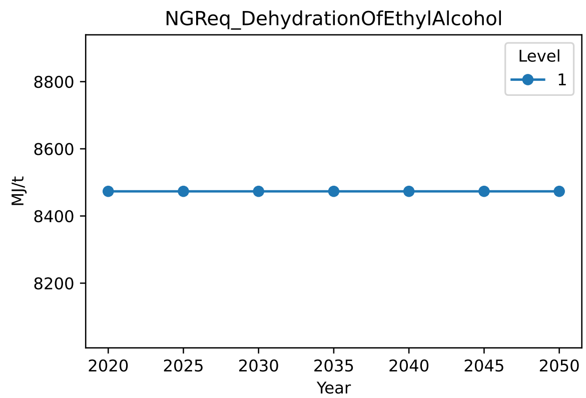
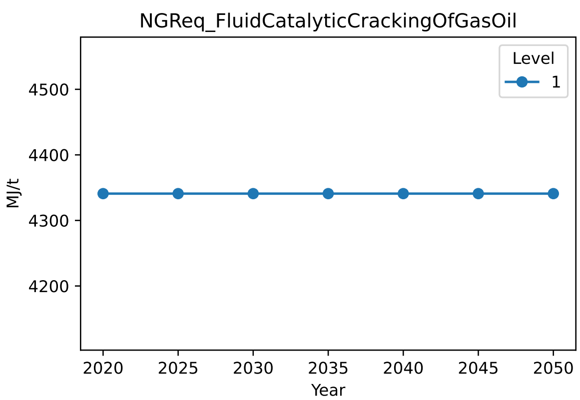
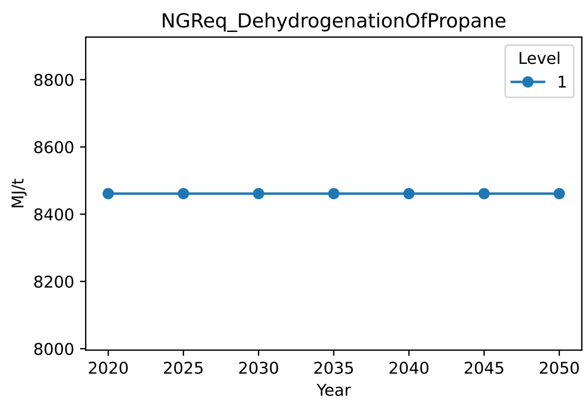
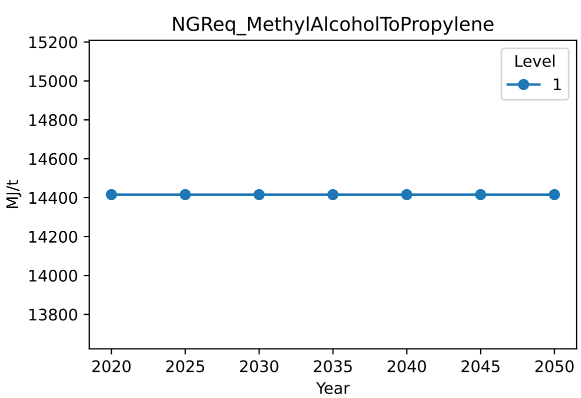
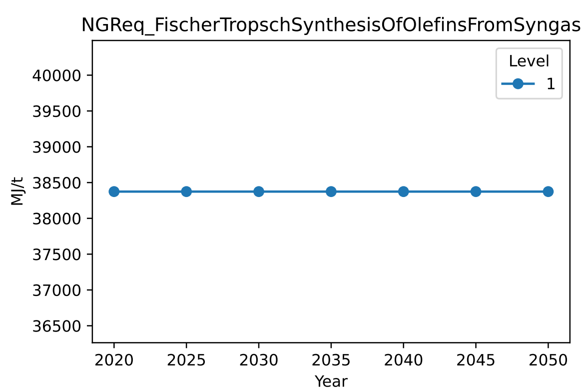
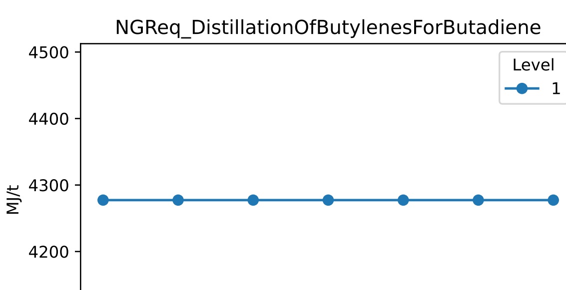
This lever sets the baseline values for natural gas utility requirements for all processes.

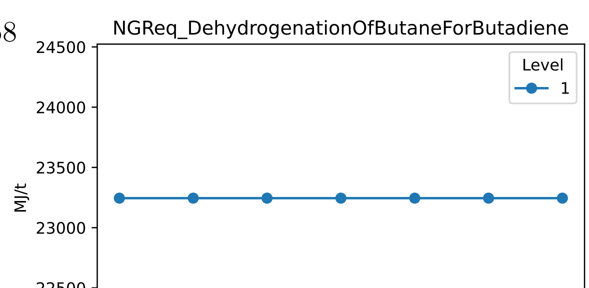
Data was sourced from Zhao et al. (2021), Jiang et al. (2020), Rosental et al. (2020), Oni et al. (2022), IEA (2021), and cross-checked against data from IHS (XXX) to estimate indicative natural gas requirements for each process.

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.

22.1 Parameter data

```
/opt/homebrew/Caskroom/miniconda/base/envs/cthru-calculator/lib/python3.10/site-packages/panc
  fig = self.plt.figure(figsize=self.figsize)
```


NGReq_SteamCrackingOfNaphtha
Level
1
21500
21000
20500
20000
19500
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_SteamCrackingOfEthane
Level
1
15000
14800
14600
14400
14200
14000
13800
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_MethylAlcoholToOlefins
Level
1
9200
9000
8800
8600
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_DehydrationOfEthylAlcohol
Level
1
8800
8600
8400
8200
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_FluidCatalyticCrackingOfGasOil
Level
1
4500
4400
4300
4200
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_DehydrogenationOfPropane
Level
1
8800
8600
8400
8200
8000
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_MethylAlcoholToPropylene
Level
1
15200
15000
14800
14600
14400
14200
14000
13800
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_FischerTropschSynthesisOfOlefinsFromSyngas
Level
1
40000
39500
39000
38500
38000
37500
37000
36500
MJ/t
2020 2025 2030 2035 2040 2045 2050
Year

NGReq_DistillationOfButylenesForButadiene
Level
1
4500
4400
4300
4200
MJ/t


NGReq_DehydrogenationOfButaneForButadiene
Level
1
24500
24000
23500
23000
MJ/t

23 electricity_emission_factor

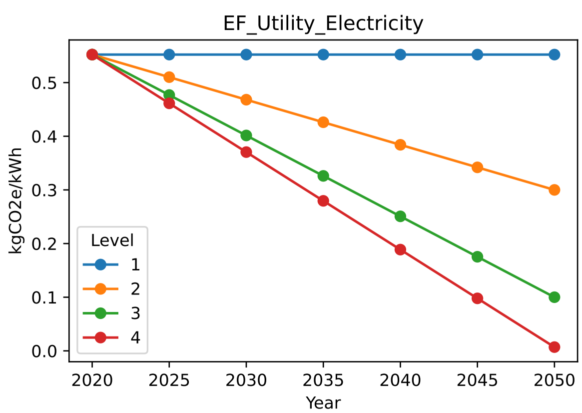
Lever ID electricity_emission_factor
Description Reduce emissions of electricity drawn from the grid
Levels

- *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_achieving_2021?**) in their plastics decarbonisation scenarios.

23.1 Parameter data



24 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

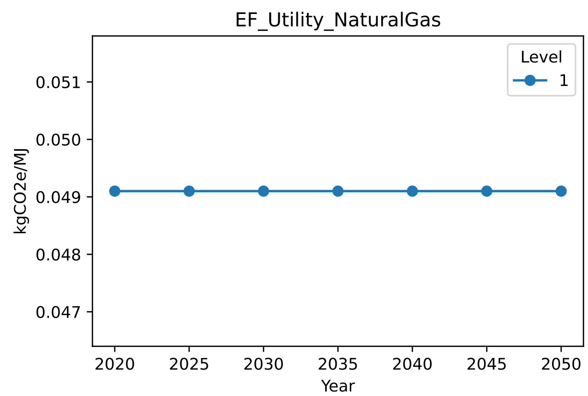
Levels

- *Level 1:* Baseline/constant

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

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

24.1 Parameter data



25 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.

25.1 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 different 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.

25.2 Biogenic carbon sequestration

Since the chemical sector can potentially act as a sink for carbon emissions (**meng_planet_2023?**) it is important to clearly model and report negative sequestered carbon from biomass feedstocks as well as positive end-of-life incineration emissions. 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.

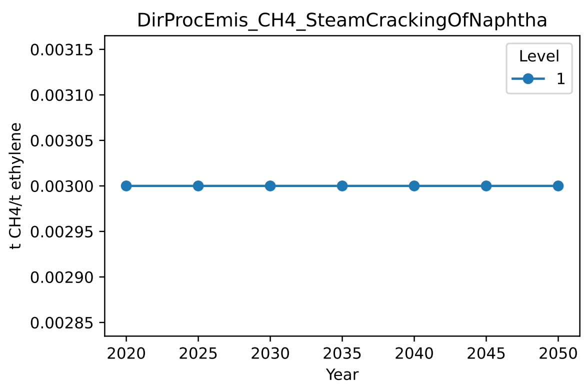
The carbon content of syngas is assumed to be 30% by mass, giving 1.1 kg CO_2 sequestered per kg syngas.

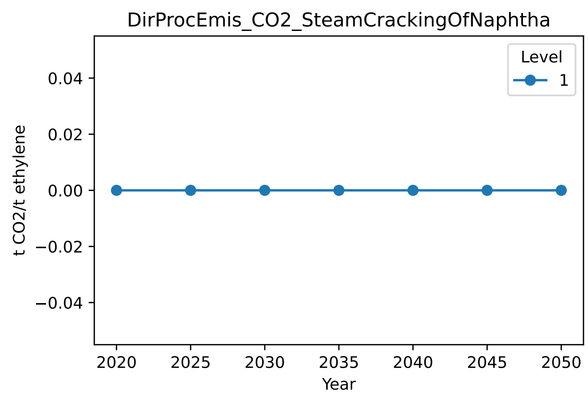
The carbon content of ethyl alcohol is assumed to be 52% by mass, giving 1.9 kg CO_2 sequestered per kg ethyl alcohol.

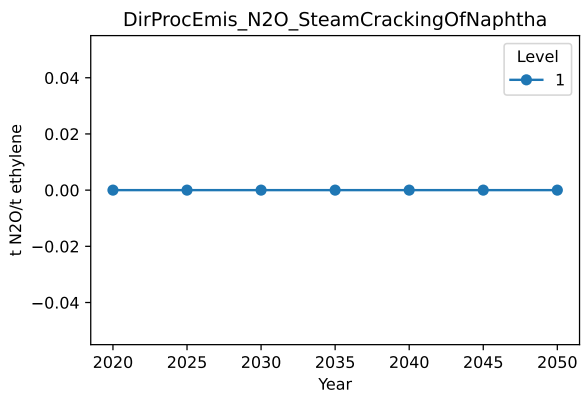
These are included as negative emissions linked to the bio-syngas and bio-ethyl-alcohol production processes.

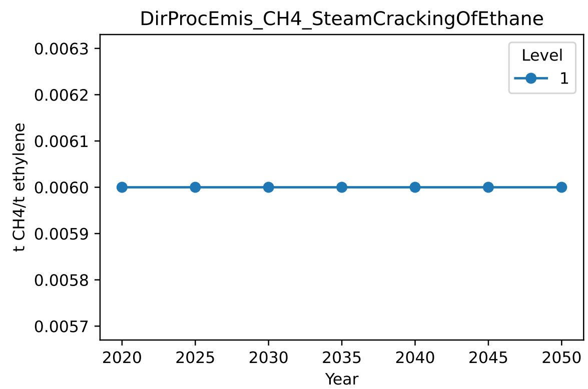
25.3 Parameter data

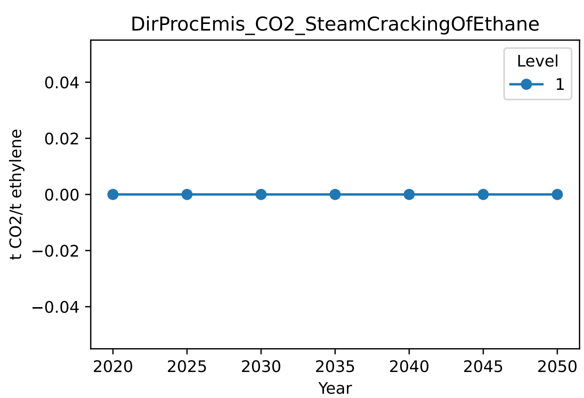
```
/opt/homebrew/Caskroom/miniconda/base/envs/cthru-calculator/lib/python3.10/site-packages/panc
  fig = self.plt.figure(figsize=self.figsize)
```

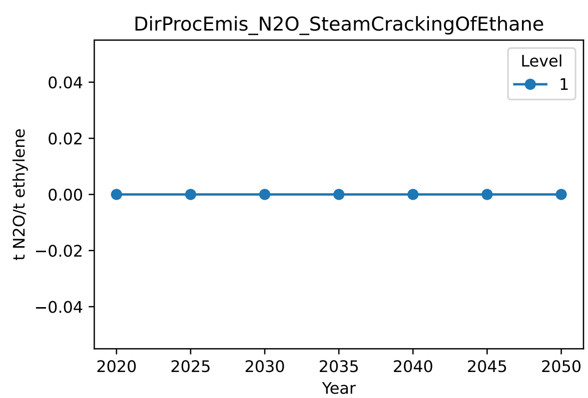

DirProcEmis_CH4_SteamCrackingOfNaphtha
Level
1
t CH4/t ethylene
0.00315
0.00310
0.00305
0.00300
0.00295
0.00290
0.00285
2020
2025
2030
2035
2040
2045
2050
Year

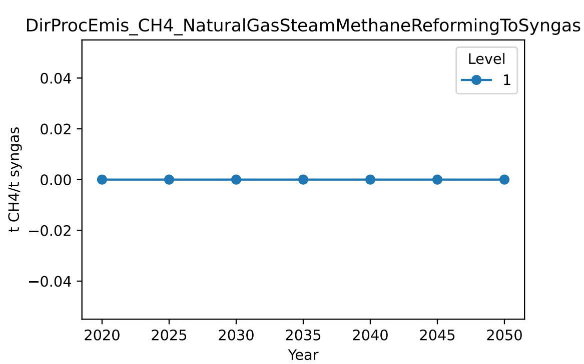

DirProcEmis_CO2_SteamCrackingOfNaphtha
Level
1
t CO2/t ethylene
0.04
0.02
0.00
−0.02
−0.04
2020
2025
2030
2035
2040
2045
2050
Year

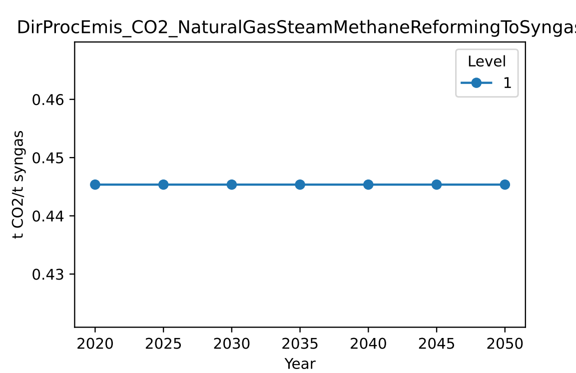

DirProcEmis_N2O_SteamCrackingOfNaphtha
Level
1
t N2O/t ethylene
0.04
0.02
0.00
−0.02
−0.04
2020
2025
2030
2035
2040
2045
2050
Year

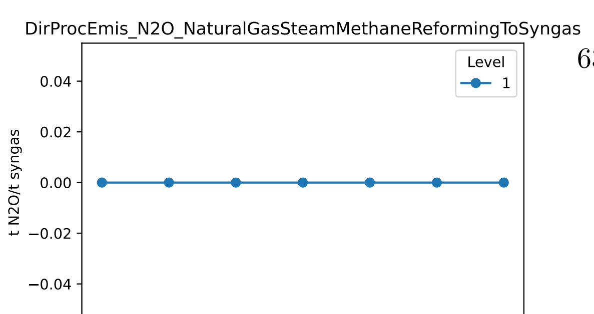

DirProcEmis_CH4_SteamCrackingOfEthane
Level
1
t CH4/t ethylene
0.0063
0.0062
0.0061
0.0060
0.0059
0.0058
0.0057
2020
2025
2030
2035
2040
2045
2050
Year

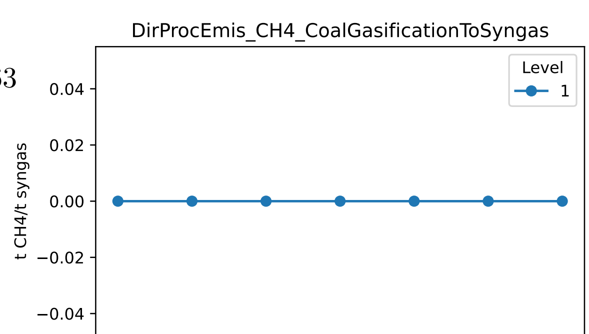

DirProcEmis_CO2_SteamCrackingOfEthane
Level
1
t CO2/t ethylene
0.04
0.02
0.00
−0.02
−0.04
2020
2025
2030
2035
2040
2045
2050
Year


DirProcEmis_N2O_SteamCrackingOfEthane
Level
1
t N2O/t ethylene
0.04
0.02
0.00
−0.02
−0.04
2020
2025
2030
2035
2040
2045
2050
Year


DirProcEmis_CH4_NaturalGasSteamMethaneReformingToSyngas
Level
1
t CH4/t syngas
0.04
0.02
0.00
−0.02
−0.04
2020
2025
2030
2035
2040
2045
2050
Year


DirProcEmis_CO2_NaturalGasSteamMethaneReformingToSyngas
Level
1
t CO2/t syngas
0.46
0.45
0.44
0.43
2020
2025
2030
2035
2040
2045
2050
Year


DirProcEmis_N2O_NaturalGasSteamMethaneReformingToSyngas
Level
1
t N2O/t syngas
0.04
0.02
0.00
−0.02
−0.04


DirProcEmis_CH4_CoalGasificationToSyngas
Level
1
t CH4/t syngas
0.04
0.02
0.00
−0.02
−0.04

26 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

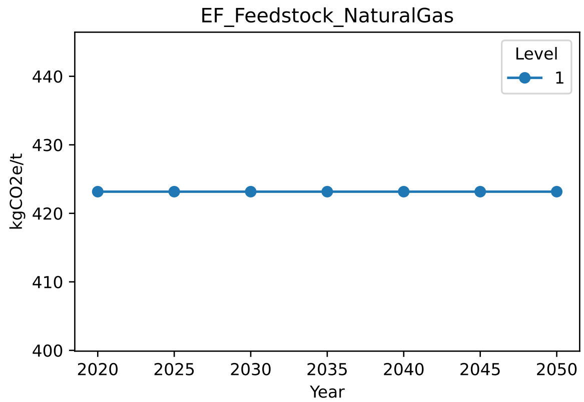
This lever controls the emissions factor for upstream production of the feedstocks that enter the model.

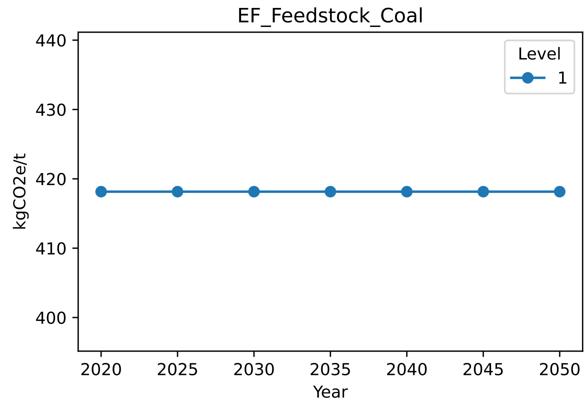
Emissions factors for natural gas, coal, gas oil, propane and butane were taken from DEFRA (2023) scope 3 emissions factors data.

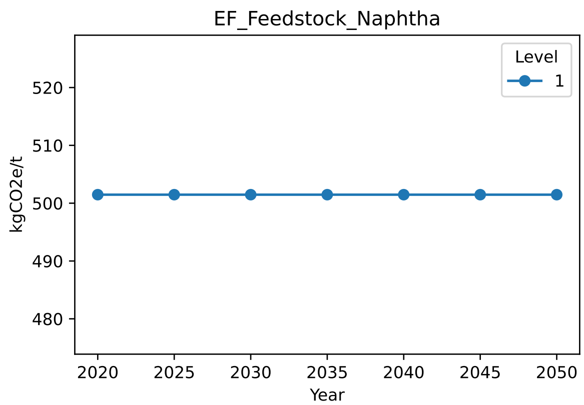
Approximate emissions factors for naphtha and ethane supply were based on the study by Nanthachatchavankul et al. (2011) for ethylene production in Thailand.

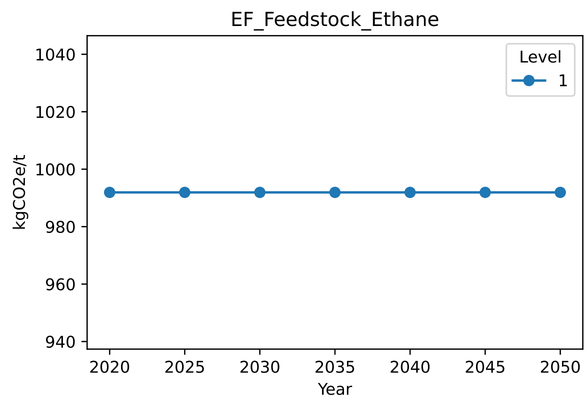
Biomass feedstocks are from Yuttitham et al. (2018) for sugarcane production in Thailand, and Farag et al. (2018) for corn production in Egypt. Crop residues are represented by DEFRA (2023) scope 3 emissions for generic straw/grass biomass.

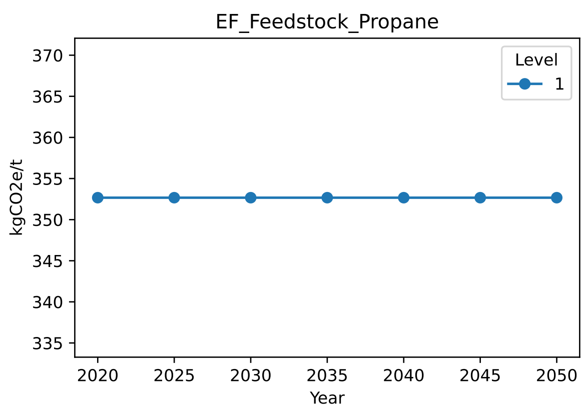
26.1 Parameter data

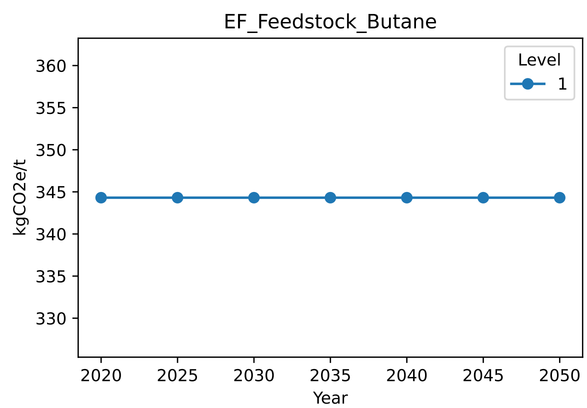

EF_Feedstock_NaturalGas
Level
1
kgCO2e/t
Year

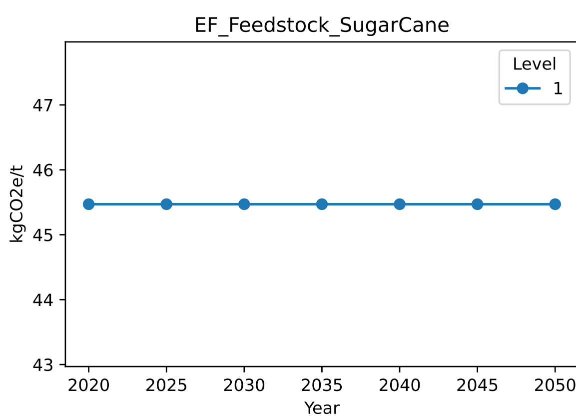

EF_Feedstock_Coal
Level
1
kgCO2e/t
Year

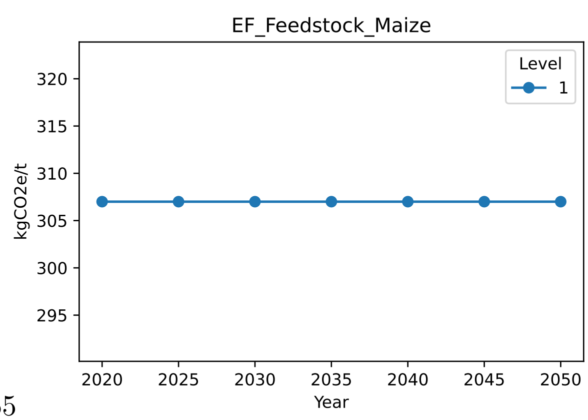

EF_Feedstock_Naphtha
Level
1
kgCO2e/t
Year

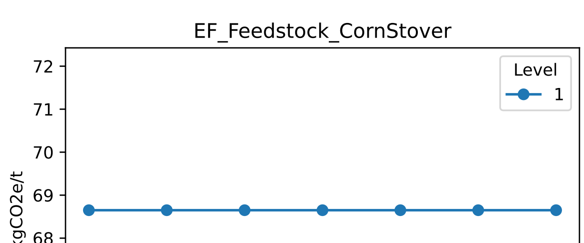

EF_Feedstock_Ethane
Level
1
kgCO2e/t
Year

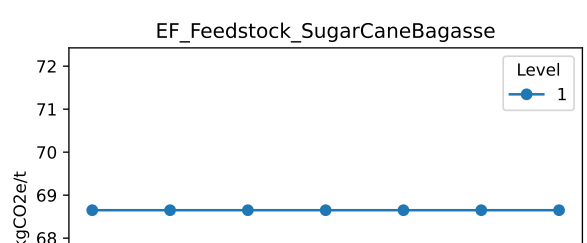

EF_Feedstock_Propane
Level
1
kgCO2e/t
Year


EF_Feedstock_Butane
Level
1
kgCO2e/t
Year


EF_Feedstock_SugarCane
Level
1
kgCO2e/t
Year


EF_Feedstock_Maize
Level
1
kgCO2e/t
Year


EF_Feedstock_CornStover
Level
1


EF_Feedstock_SugarCaneBagasse
Level
1

27 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

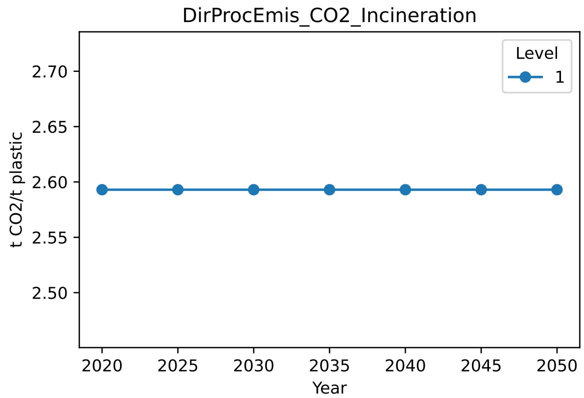
This lever controls the emissions factors for end-of-life final treatments.

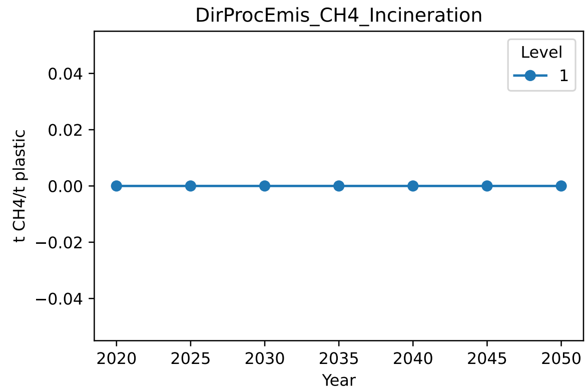
Emissions from incineration are based on data from Vlasopoulos et al. (2023) for incineration of mixed plastic waste in Europe.

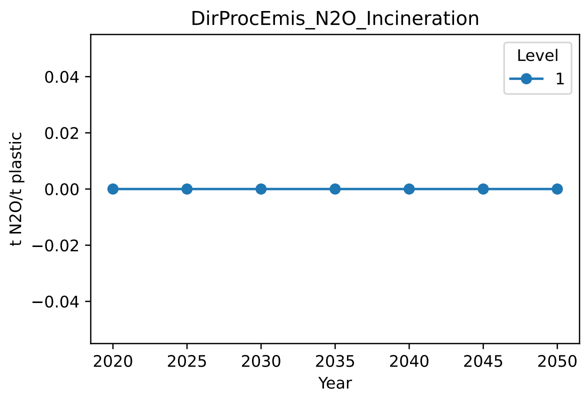
Emissions from landfilling are based on data from OECD (2023) for sanitary landfill, global scope.

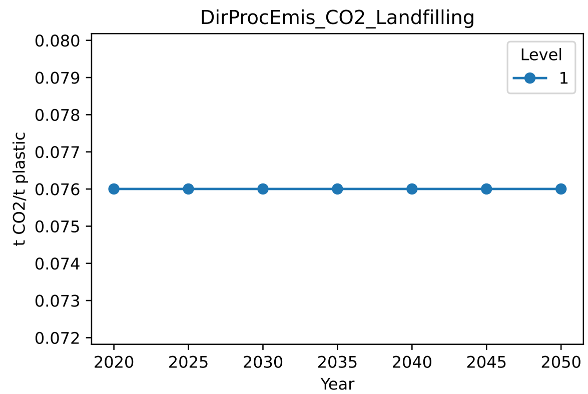
According to OECD (2022), mismanaged waste is "Waste that is not captured by any state-of-the-art waste collection or treatment facilities. It includes waste that is burned in open pits, dumped into seas or open waters, or disposed of in unsanitary landfills and dumpsites." Emissions are assumed to be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

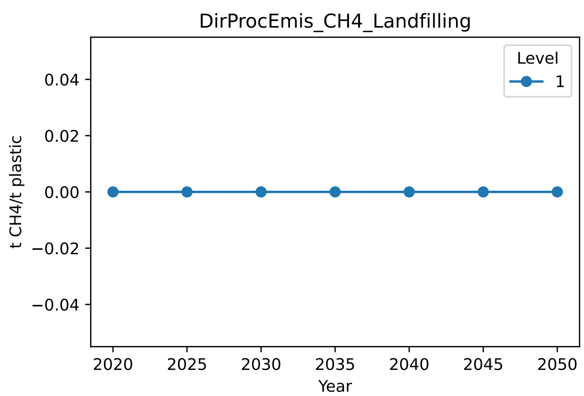
27.1 Parameter data

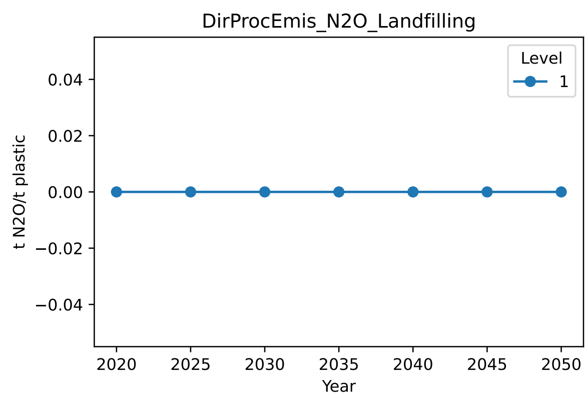

DirProcEmis_CO2_Incineration
t CO2/t plastic
2.70
2.65
2.60
2.55
2.50
2020 2025 2030 2035 2040 2045 2050
Year
Level
1

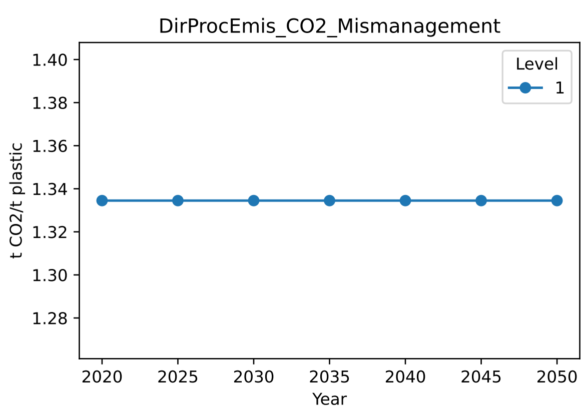

DirProcEmis_CH4_Incineration
t CH4/t plastic
0.04
0.02
0.00
−0.02
−0.04
2020 2025 2030 2035 2040 2045 2050
Year
Level
1

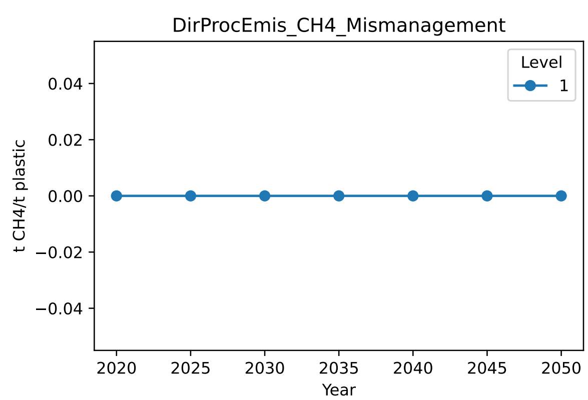

DirProcEmis_N2O_Incineration
t N2O/t plastic
0.04
0.02
0.00
−0.02
−0.04
2020 2025 2030 2035 2040 2045 2050
Year
Level
1

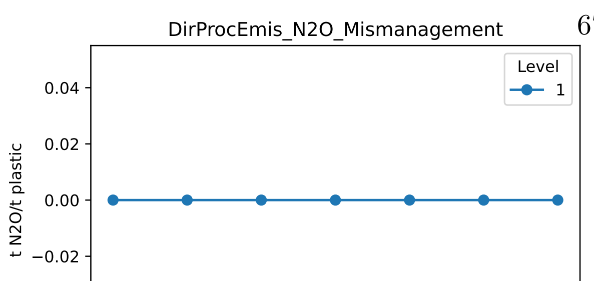

DirProcEmis_CO2_Landfilling
t CO2/t plastic
0.080
0.079
0.078
0.077
0.076
0.075
0.074
0.073
0.072
2020 2025 2030 2035 2040 2045 2050
Year
Level
1


DirProcEmis_CH4_Landfilling
t CH4/t plastic
0.04
0.02
0.00
−0.02
−0.04
2020 2025 2030 2035 2040 2045 2050
Year
Level
1


DirProcEmis_N2O_Landfilling
t N2O/t plastic
0.04
0.02
0.00
−0.02
−0.04
2020 2025 2030 2035 2040 2045 2050
Year
Level
1


DirProcEmis_CO2_Mismanagement
t CO2/t plastic
1.40
1.38
1.36
1.34
1.32
1.30
1.28
2020 2025 2030 2035 2040 2045 2050
Year
Level
1


DirProcEmis_CH4_Mismanagement
t CH4/t plastic
0.04
0.02
0.00
−0.02
−0.04
2020 2025 2030 2035 2040 2045 2050
Year
Level
1


DirProcEmis_N2O_Mismanagement
t N2O/t plastic
0.04
0.02
0.00
−0.02
Level
1

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