PyPSA-Eur-Sec Documentation

*Release 0.7.0*

author

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PyPSA-Eur-Sec is an open model dataset of the European energy system at the transmission network level that covers the full ENTSO-E area.

PyPSA-Eur-Sec builds on the electricity generation and transmission model PyPSA-Eur to add demand and supply for the following sectors: transport, space and water heating, biomass, energy consumption in the agriculture, industry and industrial feedstocks, carbon management, carbon capture and usage/sequestration. This completes the energy system and includes all greenhouse gas emitters except waste management, agriculture, forestry and land use.

WARNING: PyPSA-Eur-Sec is under active development and has several limitations which you should understand before using the model. The github repository issues collect known topics we are working on (please feel free to help or make suggestions). The documentation remains somewhat patchy. We cannot support this model if you choose to use it.

Note: You can find showcases of the model's capabilities in the Supplementary Materials of the preprint Benefits of a Hydrogen Network in Europe, the Supplementary Materials of the paper in Joule with a description of the industry sector, or in a 2021 presentation at EMP-E.

This diagram gives an overview of the sectors and the links between them:
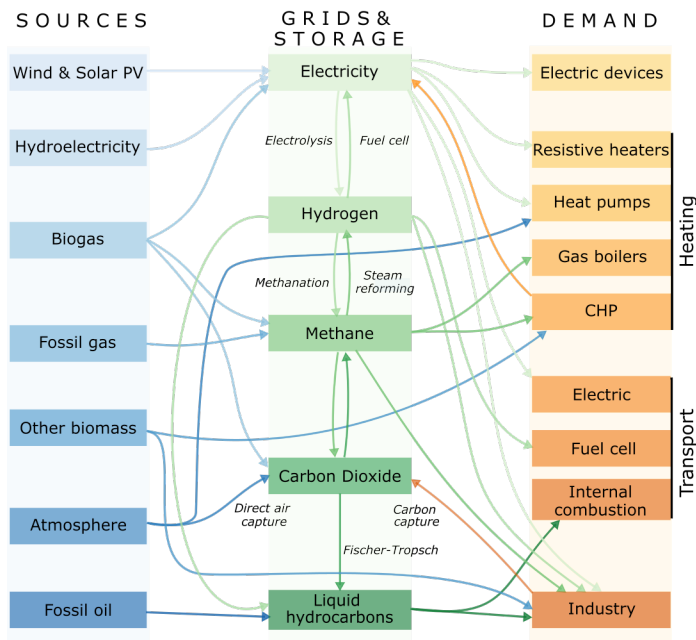
PyPSA-Eur-Sec was initially based on the model PyPSA-Eur-Sec-30 described in the paper Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system (2018) but it differs by being based on the higher resolution electricity transmission model PyPSA-Eur rather than a one-node-per-country model, and by including biomass, industry, industrial feedstocks, aviation, shipping, better carbon management, carbon capture and usage/sequestration, and gas networks.

PyPSA-Eur-Sec includes PyPSA-Eur as a snakemake subworkflow. PyPSA-Eur-Sec uses PyPSA-Eur to build the clustered transmission model along with wind, solar PV and hydroelectricity potentials and time series. Then PyPSA-Eur-Sec adds other conventional generators, storage units and the additional sectors.

Currently the scripts to solve and process the resulting PyPSA models are also included in PyPSA-Eur-Sec, although they could in future be better integrated with the corresponding scripts in PyPSA-Eur. A stumbling block to sharing solve_network.py between PyPSA-Eur and PyPSA-Eur-Sec is the different extra_functionality required to build storage and CHP constraints.

PyPSA-Eur-Sec is designed to be imported into the open toolbox PyPSA for which documentation is available as well.

This project is currently maintained by the Department of Digital Transformation in Energy Systems at the Technical University of Berlin. Previous versions were developed by the Energy System Modelling group at the Institute for Automation and Applied Informatics at the Karlsruhe Institute of Technology which was funded by the Helmholtz Association, and by the Renewable Energy Group at FIAS to carry out simulations for the CoNDyNet project, financed by the German Federal Ministry for Education and Research (BMBF) as part of the Stromnetze Research Initiative.

Workflow Outline

Note: The graph above was generated using `snakemake --rulegraph -F | sed -n "/digraph/,/}/p" | dot -Tpng -o workflow.png`

Documentation

Getting Started

- *Installation*

2.1 Installation

The subsequently described installation steps are demonstrated as shell commands, where the path before the `%` sign denotes the directory in which the commands following the `%` should be entered.

2.1.1 Install PyPSA-Eur and its data

First install PyPSA-Eur and all its dependencies. Clone the repository:

```
projects % git clone https://github.com/PyPSA/pypsa-eur.git
```

then download and unpack all the PyPSA-Eur data files by running the following snakemake rule:

```
projects/pypsa-eur % snakemake -j 1 retrieve_databundle
```

2.1.2 Clone PyPSA-Eur-Sec repository

Create a parallel directory for PyPSA-Eur-Sec with:

```
projects % git clone https://github.com/PyPSA/pypsa-eur-sec.git
```

2.1.3 Environment/package requirements

The requirements are the same as PyPSA-Eur. For `solve_network.py` in addition you need `gurobipy`. If you have xarray version >= 0.15.1, you will need the latest master branch of atlite version 0.0.2.

You can create an environment using the environment.yaml file in pypsa-eur/envs:

```
.../pypsa-eur % conda env create -f envs/environment.yaml

.../pypsa-eur % conda activate pypsa-eur
```

See details in PyPSA-Eur Installation

2.1.4 Data requirements

Small data files are included directly in the git repository, while larger ones are archived in a data bundle on zenodo (10.5281/zenodo.5824485). The data bundle's size is around 640 MB.

To download and extract the data bundle on the command line:

```
projects/pypsa-eur-sec/data % wget "https://zenodo.org/record/5824485/files/pypsa-eur-
↪sec-data-bundle.tar.gz"
projects/pypsa-eur-sec/data % tar -xvzf pypsa-eur-sec-data-bundle.tar.gz
```

The data licences and sources are given in the following table.

description	file/folder	licence	source		
JRC IDEES database	jrc-idees-2015/	CC BY 4.0	https://ec.europa.eu/jrc/en/potencia/jrc-idees		
urban/rural fraction	urban_percent.csv	unknown	unknown		
JRC biomass potentials	biomass/	unknown	https://doi.org/10.2790/39014		
JRC ENSPRESO biomass potentials	remote	CC BY 4.0	https://data.jrc.ec.europa.eu/dataset/ 74ed5a04-7d74-4807-9eab-b94774309d9f		
EEA emission statistics	eea/UNFCCC_v23.csv	EEA standard re-use policy	https://www.eea.europa.eu/data-and-maps/data/ national-emissions-reported-to-the-unfccc-and-to-the-eu-greenhouse-ga		
Eurostat Energy Balances	eurostat-energy_balances-*/	Eurostat	https://ec.europa.eu/eurostat/web/energy/data/ energy-balances		
Swiss energy statistics from Swiss Federal Office of Energy	switzerland-sfoe/	unknown	http://www.bfe.admin.ch/themen/00526/00541/ 00542/02167/index.html?dossier_id=02169		
BASt emobility statistics	emobility/	unknown	http://www.bast.de/DE/Verkehrstechnik/ Fachthemen/v2-verkehrszaehlung/Stundenwerte. html?nn=626916		
BDEW heating profile	heat_load_profile_BDEW.csv	unknown	https://github.com/oemof/demandlib		
heating profiles for Aarhus	heat_load_profile_DK_AdamJensen.csv	unknown	Adam Jensen MA thesis at Aarhus University		
George Lavidas wind/wave costs	Wind-WaveWEC_GLTB.xlsx	unknown	George Lavidas		
country codes	Country_codes.csv	CC BY 4.0	Marta Victoria		
co2 budgets	co2_budget.csv	CC BY 4.0	https://arxiv.org/abs/2004.11009		
existing heating potentials	existing_infrastructure/existing_heating_raw.csv	unknown	https://ec.europa.eu/energy/studies/ mapping-and-analyses-current-and-future-2020-2030-heatingcooling-fu en?redir=1		
IRENA existing VRE capacities	existing_infrastructure/{solar|onwind|offwind}_capcity_IRENA.csv	unknown	https://www.irena.org/Statistics/Download-Data		
USGS ammonia production	myb1-2017-nitro.xls	unknown	https://www.usgs.gov/centers/nmic/ nitrogen-statistics-and-information		
hydrogen salt cavern potentials	h2_salt_caverns_GWh_per_sqkm.geojson	CC BY 4.0	https://doi.org/10.1016/j.ijhydene.2019.12.161 https://doi.org/10.20944/preprints201910.0187. v1		
international port trade volumes	attributed_ports.json	CC BY 4.0	https://datacatalog.worldbank.org/search/dataset/0038118/Global—Intern Ports		
hotmaps industrial site database	Industrial_Database.csv	CC BY 4.0	https://gitlab.com/hotmaps/industrial_sites/ industrial_sites_Industrial_Database		
Hotmaps building stock data	data_building_stock.csv	CC BY 4.0	https://gitlab.com/hotmaps/building-stock		
U-values Poland	u_values_poland.csv	unknown	https://data.europa.eu/euodp/de/data/dataset/ building-stock-observatory		
Floor area missing in hotmaps building stock data	floor_area_missing.csv	unknown	https://data.europa.eu/euodp/de/data/dataset/ building-stock-observatory		
Comparative level investment	comparative_level_investment.csv	Eurostat	https://ec.europa.eu/eurostat/statistics-explained/ index.php?title=Comparative_price_levels_for_ investment		
Electricity taxes	electricity_taxes_eu.csv	Eurostat	https://appsso.eurostat.ec.europa.eu/nui/show.do? dataset=nrg_pc_204&lang=en		
Building topologies	tabula-calculator-	un-	https://episcope.eu/fileadmin/tabula/public/calc/		

2.1. Installation **7**

2.1.5 Set up the default configuration

First make your own copy of the `config.yaml` based on `config.default.yaml`. For example:

```
projects/pypsa-eur-sec % cp config.default.yaml config.yaml
```

2.1.6 Getting started

In `config.yaml` you can control the settings for the scenarios you want to run, such as the number of nodes, the CO2 limit, the installable potentials for solar and wind, which technologies are activated, etc.

To run the full optimization with your settings:

```
projects/pypsa-eur-sec % snakemake -j1
```

Warning: you may need a computer cluster for this (with e.g. 10-100 GB of RAM and several processors).

To only prepare the networks, you can run the scripts up to the point before optimization:

```
projects/pypsa-eur-sec % snakemake -j1 prepare_sector_networks
```

Implementation details

- *Spatial resolution*
- *Supply and demand*
- *Technology and cost assumptions*

2.2 Spatial resolution

The default nodal resolution of the model follows the electricity generation and transmission model PyPSA-Eur, which clusters down the electricity transmission substations in each European country based on the k-means algorithm (See cluster_network for a complete explanation). This gives nodes which correspond to major load and generation centres (typically cities).

The total number of nodes for Europe is set in the `config.yaml` file under `clusters`. The number of nodes can vary between 37, the number of independent countries / synchronous areas, and several hundred. With 200-300 nodes the model needs 100-150 GB RAM to solve with a commercial solver like Gurobi.

Exemplary unsolved network clustered to 512 nodes:
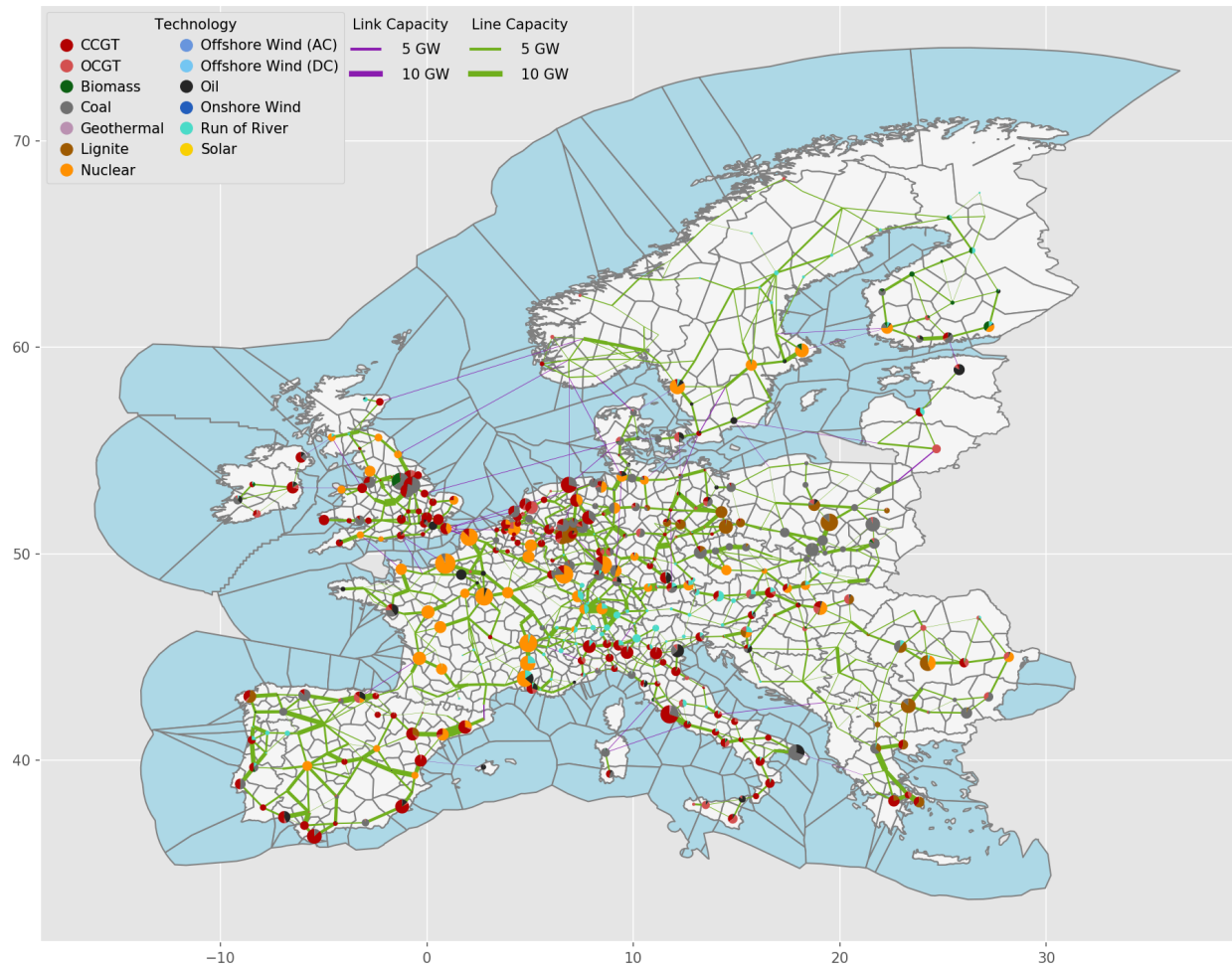
Exemplary unsolved network clustered to 37 nodes:
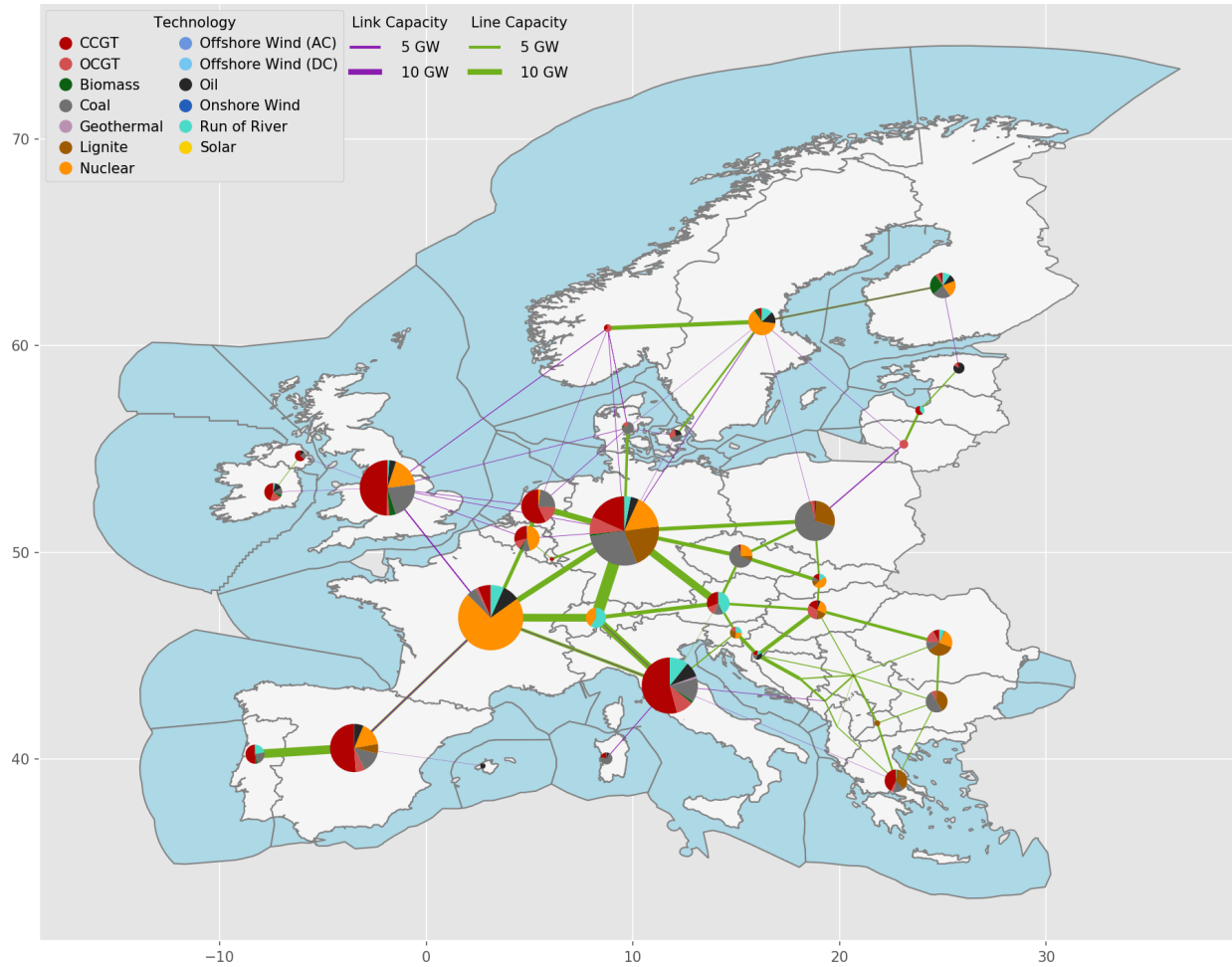
The total number of nodes for Europe is set in the config.yaml file under clusters. The number of nodes can vary between 37, the number of independent countries/synchronous areas, and several hundred. With 200-300 nodes, the model needs 100-150 GB RAM to solve with a commercial solver like Gurobi. Not all of the sectors are at the full nodal resolution, and some demand for some sectors is distributed to nodes using heuristics that need to be corrected. Some networks are copper-plated to reduce computational times.

Here are some examples of how spatial resolution is set for different sectors in PyPSA-Eur-Sec:

- Electricity network: Modeled as nodal.

- Electricity residential and commercial demand: Modeled as nodal, distributed in each country based on population and GDP.

- Electricity distribution network: Not included in the model, but a link per node can be used to represent energy transferred between distribution and transmission levels (explained more in detail below).

- Residential and commercial building heating demand: Modeled as nodal, distributed in each country based on population.

- Electricity demand in industry: Modeled as nodal, based on the location of industrial facilities from HotMaps database.

- Industry demand (heat, chemicals, etc.) : Modeled as nodal, distributed in each country based on locations of industry from HotMaps database.

- Hydrogen network: Modeled as nodal (if activated in the config file).

- Methane network: It can be modeled as a single node for Europe or it can be nodally resolved if activated in the config. One node can be considered reasonable since future demand is expected to be low and no bottlenecks are expected. Also, the nodally resolved methane grid is based on SciGRID_gas data.

- Solid biomass: It can be modeled as a single node for Europe or it can be nodally resolved if activated in the config. Nodal modeling includes modeling biomass potential per country (given per country, then distributed by population density within) and the transport of solid biomass between countries.

- CO2: It can be modeled as a single node for Europe or it can be nodally resolved with CO2 transport pipelines if activated in the config. It should mentioned that in single node mode a transport and storage cost is added for sequestered CO2, the cost of which can be adjusted in the config.

- Liquid hydrocarbons: Modeled as a single node for Europe, since transport costs for liquids are low and no bottlenecks are expected.

Electricity distribution network

Contrary to the transmission grid, the grid topology at the distribution level (at and below 110 kV) is not included due to the very high computational burden. However, a link per node can be used (if activated in the Config file) to represent energy transferred between distribution and transmission levels at every node. In essence, the total energy capacity connecting the transmission grid and the low-voltage level is optimized. The cost assumptions for this link can be adjusted in Config file options , and is currently assumed to be 500 Eur/kW.

Rooftop PV, heat pumps, resistive heater, home batteries chargers for passenger EVs, as well as individual heating technologies (heat pumps and resistive heaters) are connected to low-voltage level. All the remaining generation and storage technologies are connected to the transmission grid. In practice, this means that the distribution grid capacity is only extended if it is necessary to balance the mismatch between local generation and demand.

2.3 Supply and demand

An initial orientation to the supply and demand options in the model PyPSA-Eur-Sec can be found in the description of the model PyPSA-Eur-Sec-30 in the paper Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system (2018). The latest version of PyPSA-Eur-Sec differs by including biomass, industry, industrial feedstocks, aviation, shipping, better carbon management, carbon capture and usage/sequestration, and gas networks.

The basic supply (left column) and demand (right column) options in the model are described in this figure:
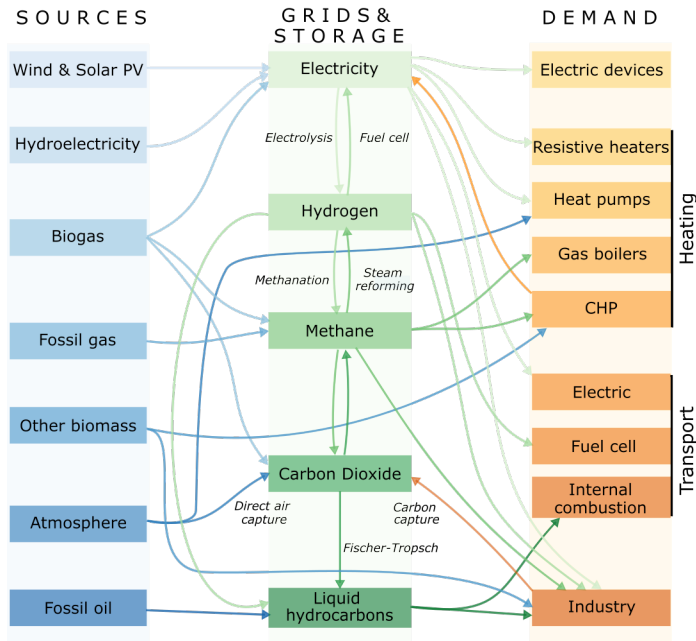
2.3.1 Electricity supply and demand

Electricity supply and demand follows the electricity generation and transmission model PyPSA-Eur, except that hydrogen storage is integrated into the hydrogen supply, demand and network, and PyPSA-Eur-Sec includes CHPs.

Unlike PyPSA-Eur, PyPSA-Eur-Sec does not distribution electricity demand for industry according to population and GDP, but uses the geographical data from the Hotmaps Industrial Database.

Also unlike PyPSA-Eur, PyPSA-Eur-Sec subtracts existing electrified heating from the existing electricity demand, so that power-to-heat can be optimised separately.

The remaining electricity demand for households and services is distributed inside each country proportional to GDP and population.

2.3.2 Heat demand

Building heating in residential and services sectors is resolved regionally, both for individual buildings and district heating systems, which include different supply options (see *Heat supply*.) Annual heat demands per country are retrieved from JRC-IDEES and split into space and water heating. For space heating, the annual demands are converted to daily values based on the population-weighted Heating Degree Day (HDD) using the atlite tool, where space heat demand is proportional to the difference between the daily average ambient temperature (read from ERA5) and a threshold temperature above which space heat demand is zero. A threshold temperature of 15 °C is assumed by default. The daily space heat demand is distributed to the hours of the day following heat demand profiles from BDEW. These differ for weekdays and weekends/holidays and between residential and services demand.

Space heating

The space heating demand can be exogenously reduced by retrofitting measures that improve the buildings' thermal envelopes.

```
  MWh_MeOH_per_MWh_e: 3.6907 # in LHV, source: DECHEMA (2017): Low carbon energy and
→feedstock for the European chemical industry , pg. 64.
```

Co-optimsing of building renovation is also possible, if it is activated in the config file. Renovation of the thermal envelope reduces the space heating demand and is optimised at each node for every heat bus. Renovation measures through additional insulation material and replacement of energy inefficient windows are considered. In a first step, costs per energy savings are estimated in build_retro_cost.py. They depend on the insulation condition of the building stock and costs for renovation of the building elements. In a second step, for those cost per energy savings two possible renovation strengths are determined: a moderate renovation with lower costs, a lower maximum possible space heat savings, and an ambitious renovation with associated higher costs and higher efficiency gains. They are added by step-wise linearisation in form of two additional generations in prepare_sector_network.py. Further information are given in the publication :

> Mitigating heat demand peaks in buildings in a highly renewable European energy system, (2021).

Water heating

Hot water demand is assumed to be constant throughout the year.

Urban and rural heating

For every country, heat demand is split between low and high population density areas. These country-level totals are then distributed to each region in proportion to their rural and urban populations respectively. Urban areas with dense heat demand can be supplied with large-scale district heating systems. The percentage of urban heat demand that can be supplied by district heating networks as well as lump-sum losses in district heating systems is exogenously determined in the config file.

Cooling demand

Cooling is electrified and is included in the electricity demand. Cooling demand is assumed to remain at current levels. An example of regional distribution of the total heat demand for network 181 regions is depicted below.
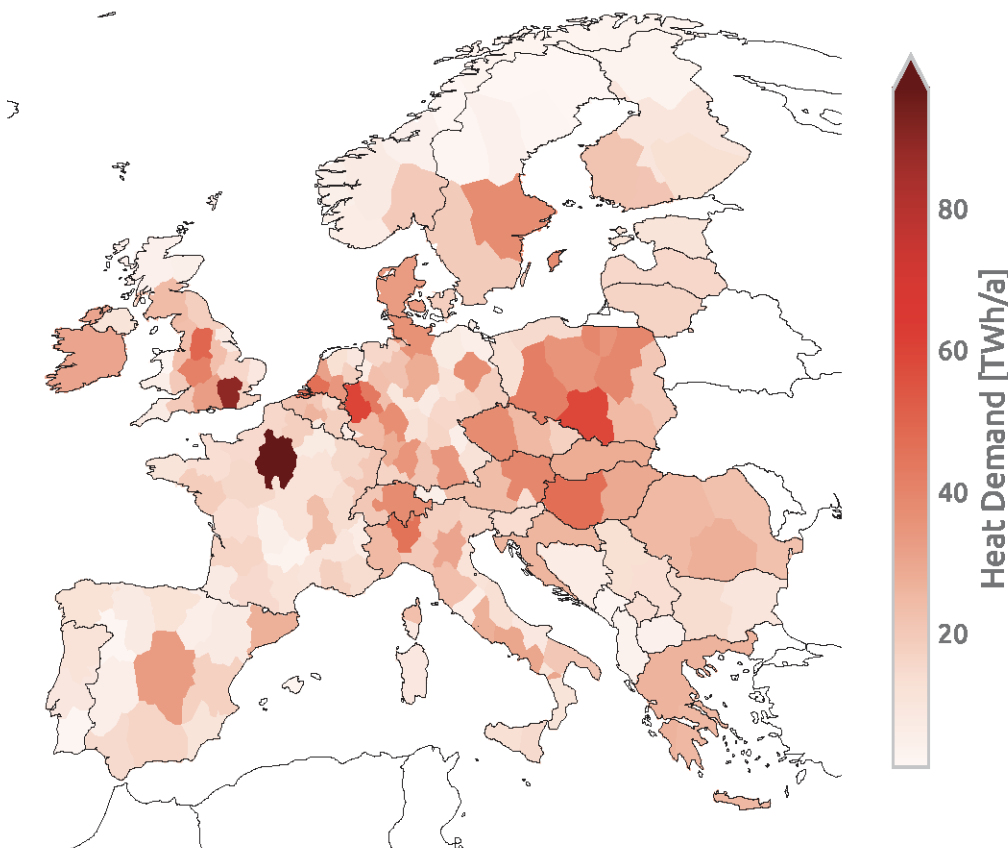
As below figure shows, the current total heat demand in Europe is similar to the total electricity demand but features much more pronounced seasonal variations. The current total building heating demand in Europe adds up to 3084 TWh/a of which 78% occurs in urban areas.
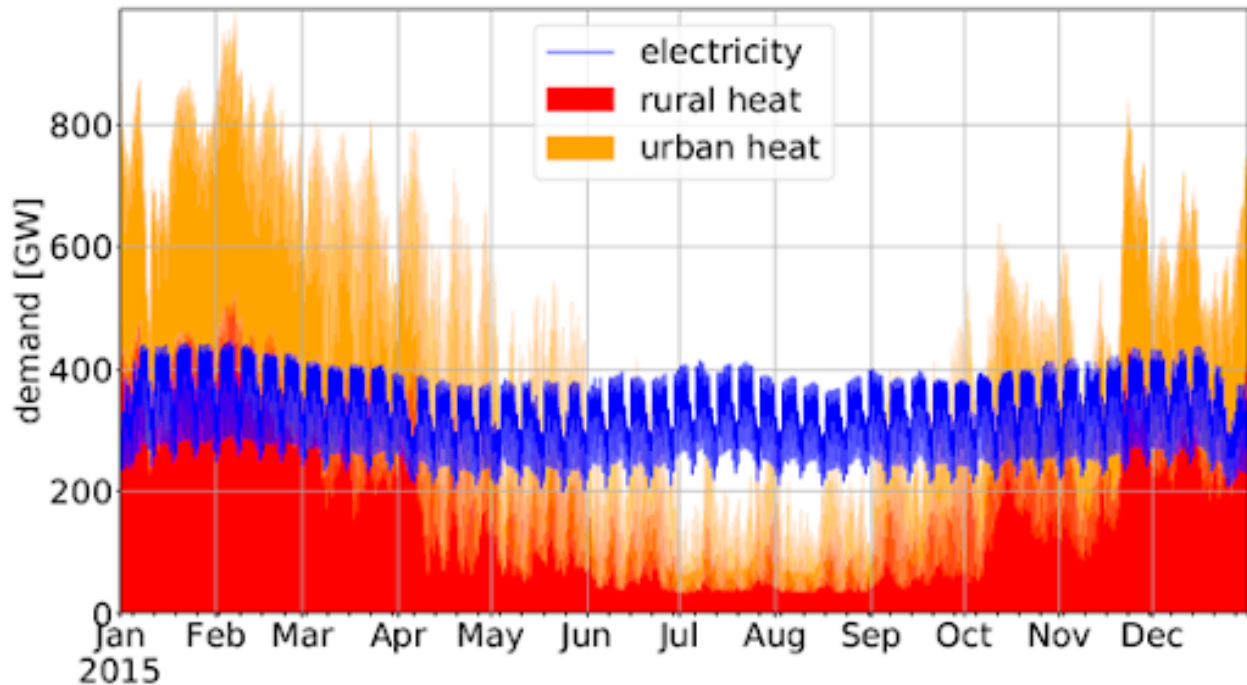
In practice, in PyPSA-Eur-Sec, there are heat demand buses to which the corresponding heat demands are added.

1) Urban central heat: large-scale district heating networks in urban areas with dense heat population. Residential and services demand in these areas are added as demands to this bus

2) Residential urban decentral heat: heating for residential buildings in urban areas not using district heating

3) Services urban decentral heat: heating for services buildings in urban areas not using district heating

4) Residential rural heat: heating for residential buildings in rural areas with low population density.

5) Services rural heat: heating for residential services buildings in rural areas with low population density. Heat demand from agriculture sector is also included here.

2.3.3 Heat supply

Different supply options are available depending on whether demand is met centrally through district heating systems, or decentrally through appliances in individual buildings.

Urban central heat

For large-scale district heating systems the following options are available: combined heat and power (CHP) plants consuming gas or biomass from waste and residues with and without carbon capture (CC), large-scale air-sourced heat pumps, gas and oil boilers, resistive heaters, and fuel cell CHPs. Additionally, waste heat from the Fischer-Tropsch and Sabatier processes for the production of synthetic hydrocarbons can supply district heating systems. For more detailed explanation of these processes, see *Oil-based products supply* and *Methane supply*.

Residential and Urban decentral heat

Supply options in individual buildings include gas and oil boilers, air- and ground-sourced heat pumps, resistive heaters, and solar thermal collectors. Ground-source heat pumps are only allowed in rural areas because of space constraints. Thus, only air- source heat pumps are allowed in urban areas. This is a conservative assumption, since

there are many possible sources of low-temperature heat that could be tapped in cities (e.g. waste water, ground water, or natural bodies of water). Costs, lifetimes and efficiencies for these technologies are retrieved from the technology-data repository.

Below are more detailed explanations for each heating supply component, all of which are modelled as links in PyPSA-Eur-Sec.

Large-scale CHP

Large Combined Heat and Power plants are included in the model if it is specified in the config file.

CHPs are based on back pressure plants operating with a fixed ratio of electricity to heat output. The efficiencies of each are given on the back pressure line, where the back pressure coefficient cb is the electricity output divided by the heat output. (For a more complete explanation of the operation of CHPs refer to the study by Dahl et al. : Cost sensitivity of optimal sector-coupled district heating production systems.

PyPSA-Eur-Sec includes CHP plants fueled by methane and solid biomass from waste and residues. Hydrogen fuel cells also produce both electricity and heat.

The methane CHP is modeled on the Danish Energy Agency (DEA) "Gas turbine simple cycle (large)" while the solid biomass CHP is based on the DEA's "09b Wood Pellets Medium". For biomass CHP, cb = 0.46 , whereas for gas CHP, cb = 1.

NB: The old PyPSA-Eur-Sec-30 model assumed an extraction plant (like the DEA coal CHP) for gas which has flexible production of heat and electricity within the feasibility diagram of Figure 4 in the study by Brown et al. We have switched to the DEA back pressure plants since these are more common for smaller plants for biomass, and because the extraction plants were on the back pressure line for 99.5% of the time anyway. The plants were all changed to back pressure in PyPSA-Eur-Sec v0.4.0.

Micro-CHP

PyPSA-Eur-Sec allows individual buildings to make use of micro gas CHPs that are assumed to be installed at the distribution grid level.

Heat pumps

The coefficient of performance (COP) of air- and ground-sourced heat pumps depends on the ambient or soil temperature respectively. Hence, the COP is a time-varying parameter (refer to Config file). Generally, the COP will be lower during winter when temperatures are low. Because the ambient temperature is more volatile than the soil temperature, the COP of ground-sourced heat pumps is less variable. Moreover, the COP depends on the difference between the source and sink temperatures:

$$\Delta T = T_{sink} T_{source}$$

For the sink water temperature Tsink we assume 55 °C [Config file]. For the time- and location-dependent source temperatures Tsource, we rely on the ERA5 reanalysis weather data. The temperature differences are converted into COP time series using results from a regression analysis performed in the study by Stafell et al.. For air-sourced heat pumps (ASHP), we use the function:

$$COP(\Delta T) = 6.81 + 0.121 \Delta T + 0.000630 \Delta T^2$$

for ground-sourced heat pumps (GSHP), we use the function:

$$COP(\Delta T) = 8.77 + 0.150 \Delta T + 0.000734 \Delta T^2$$

Resistive heaters

Can be activated in Config from the boilers option. Resistive heaters produce heat with a fixed conversion efficiency (refer to Technology-data repository).

Gas, oil, and biomass boilers

Can be activated in Config from the boilers , oil boilers , and biomass boiler option. Similar to resistive heaters, boilers have a fixed efficiency and produce heat using gas, oil or biomass.

Solar thermal collectors

Can be activated in the config file from the solar_thermal option. Solar thermal profiles are built based on weather data and also have the options for setting the sky model and the orientation of the panel in the config file, which are then used by the atlite tool to calculate the solar resource time series.

Waste heat from Fuel Cells, Methanation and Fischer-Tropsch plants

Waste heat from fuel cells in addition to processes like Fischer-Tropsch, methanation, and Direct Air Capture (DAC) is dumped into district heating networks.

Existing heating capacities and decommissioning

For the myopic transition paths, capacities already existing for technologies supplying heat are retrieved from "Mapping and analyses of the current and future (2020 - 2030)" . For the sake of simplicity, coal, oil and gas boiler capacities are assimilated to gas boilers. Besides that, existing capacities for heat resistors, air-sourced and ground-sourced heat pumps are included in the model. For heating capacities, 25% of existing capacities in 2015 are assumed to be decommissioned in every 5-year time step after 2020.

Thermal Energy Storage

Activated in Config from the tes option.

Thermal energy can be stored in large water pits associated with district heating systems and individual thermal energy storage (TES), i.e., small water tanks. Water tanks are modelled as stores. A thermal energy density of 46.8 kWh $_{th}$/m3 is assumed, corresponding to a temperature difference of 40 K. The decay of thermal energy in the stores: 1- $e^{-1/24}$ is assumed to have a time constant of τ=180 days for central TES and τ=3 days for individual TES, both modifiable through tes_tau in config file. Charging and discharging efficiencies are 90% due to pipe losses.

Retrofitting of the thermal envelope of buildings

Co-optimising building renovation is only enabled if in the config file. To reduce the computational burden, default setting is set as false.

Renovation of the thermal envelope reduces the space heating demand and is optimised at each node for every heat bus. Renovation measures through additional insulation material and replacement of energy inefficient windows are considered.

In a first step, costs per energy savings are estimated in the build_retro_cost.py script. They depend on the insulation condition of the building stock and costs for renovation of the building elements. In a second step, for those cost per energy savings two possible renovation strengths are determined: a moderate renovation with lower costs and lower maximum possible space heat savings, and an ambitious renovation with associated higher costs and higher efficiency gains. They are added by step-wise linearisation in form of two additional generations in the prepare_sector_network.py script.

Settings in the config.yaml concerning the endogenously optimisation of building renovation include cost factor, interest rate, annualised cost, tax weighting, and construction index.

Further information are given in the study by Zeyen et al. : Mitigating heat demand peaks in buildings in a highly renewable European energy system, (2021).

2.3.4 Hydrogen demand

Hydrogen is consumed in the industry sector (see *Industry demand*) to produce ammonia (see Chemicals Industry) and direct reduced iron (DRI) (see Iron and Steel). Hydrogen is also consumed to produce synthetic methane (see *Methane supply*) and liquid hydrocarbons (see *Oil-based products supply*) which have multiple uses in industry and other sectors. Hydrogen is also used for transport applications (see *Transportation*), where it is exogenously fixed. It is used in heavy-duty land transport and as liquified hydrogen in the shipping sector (see Shipping). Furthermore,

stationary fuel cells may re-electrify hydrogen (with waste heat as a byproduct) to balance renewable fluctuations (see *Electricity supply and demand*). The waste heat from the stationary fuel cells can be used in district-heating systems.

2.3.5 Hydrogen supply

Today, most of the H_2 consumed globally is produced from natural gas by steam methane reforming (SMR)

$$CH_4 + H_2O \rightarrow CO + 3H_2$$
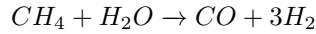
combined with a water-gas shift reaction

$$CO + H_2O \rightarrow CO_2 + H_2$$
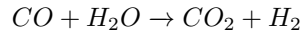
SMR is included here. PyPSA-Eur-Sec allows this route of H_2 production with and without [carbon capture (CC)] (see *Carbon dioxide capture, usage and sequestration (CCU/S)*). These routes are often referred to as blue and grey hydrogen. Here, methane input can be both of fossil or synthetic origin.

Green hydrogen can be produced by electrolysis to split water into hydrogen and oxygen

$$2H_2O \rightarrow 2H_2 + O_2$$
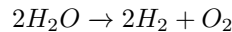
For the electrolysis, alkaline electrolysers are chosen since they have lower cost and higher cumulative installed capacity than polymer electrolyte membrane (PEM) electrolysers. The techno-economic assumptions are taken from the technology-data repository. Waste heat from electrolysis is not leveraged in the model.

Transport

Hydrogen is transported by pipelines. H_2 pipelines are endogenously generated, either via a greenfield H_2 network, or by retrofitting natural gas pipelines). Retrofitting is implemented in such a way that for every unit of decommissioned gas pipeline, a share (60% is used in the study by Neumann et al.) of its nominal capacity (exogenously determined in the config file.) is available for hydrogen transport. When the gas network is not resolved, this input denotes the potential for gas pipelines repurposed into hydrogen pipelines. New pipelines can be built additionally on all routes where there currently is a gas or electricity network connection. These new pipelines will be built where no sufficient retrofitting options are available. The capacities of new and repurposed pipelines are a result of the optimisation.

Storage

Hydrogen can be stored in overground steel tanks or underground salt caverns. For the latter, energy storage capacities in every country are limited to the potential estimation for onshore salt caverns within 50 km of shore to avoid environmental issues associated with brine solution disposal. Underground storage potentials for hydrogen in European salt caverns is acquired from Caglayan et al.

2.3.6 Methane demand

Methane is used in individual and large-scale gas boilers, in CHP plants with and without carbon capture, in OCGT and CCGT power plants, and in some industry subsectors for the provision of high temperature heat (see *Industry demand*). Methane is not used in the transport sector because of engine slippage.

2.3.7 Methane supply

In addition to methane from fossil origins, the model also considers biogenic and synthetic sources. The gas network can either be modelled, or it can be assumed that gas transport is not limited. If gas infrastructure is regionally resolved, fossil gas can enter the system only at existing and planned LNG terminals, pipeline entry-points, and intra- European gas extraction sites, which are retrieved from the SciGRID Gas IGGIELGN dataset and the GEM Wiki. Biogas can be

upgraded to methane. Synthetic methane can be produced by processing hydrogen and captures CO_2 in the Sabatier reaction

$$CO_2 + 4H_2 \rightarrow CH_4 + 2H_2O$$
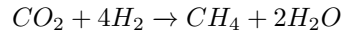
Direct power-to-methane conversion with efficient heat integration developed in the HELMETH project is also an option. The share of synthetic, biogenic and fossil methane is an optimisation result depending on the techno-economic assumptions.

Methane transport

The existing European gas transmission network is represented based on the SciGRID Gas IGGIELGN dataset. This dataset is based on compiled and merged data from the ENTSOG maps and other publicly available data sources. It includes data on the capacity, diameter, pressure, length, and directionality of pipelines. Missing capacity data is conservatively inferred from the pipe diameter following conversion factors derived from an EHB report. The gas network is clustered to the selected number of model regions. Gas pipelines can be endogenously expanded or repurposed for hydrogen transport. Gas flows are represented by a lossless transport model. Methane is assumed to be transmitted without cost or capacity constraints because future demand is predicted to be low compared to available transport capacities.

The following figure shows the unclustered European gas transmission network based on the SciGRID Gas IGGIELGN dataset. Pipelines are color-coded by estimated capacities. Markers indicate entry-points, sites of fossil resource extraction, and LNG terminals.
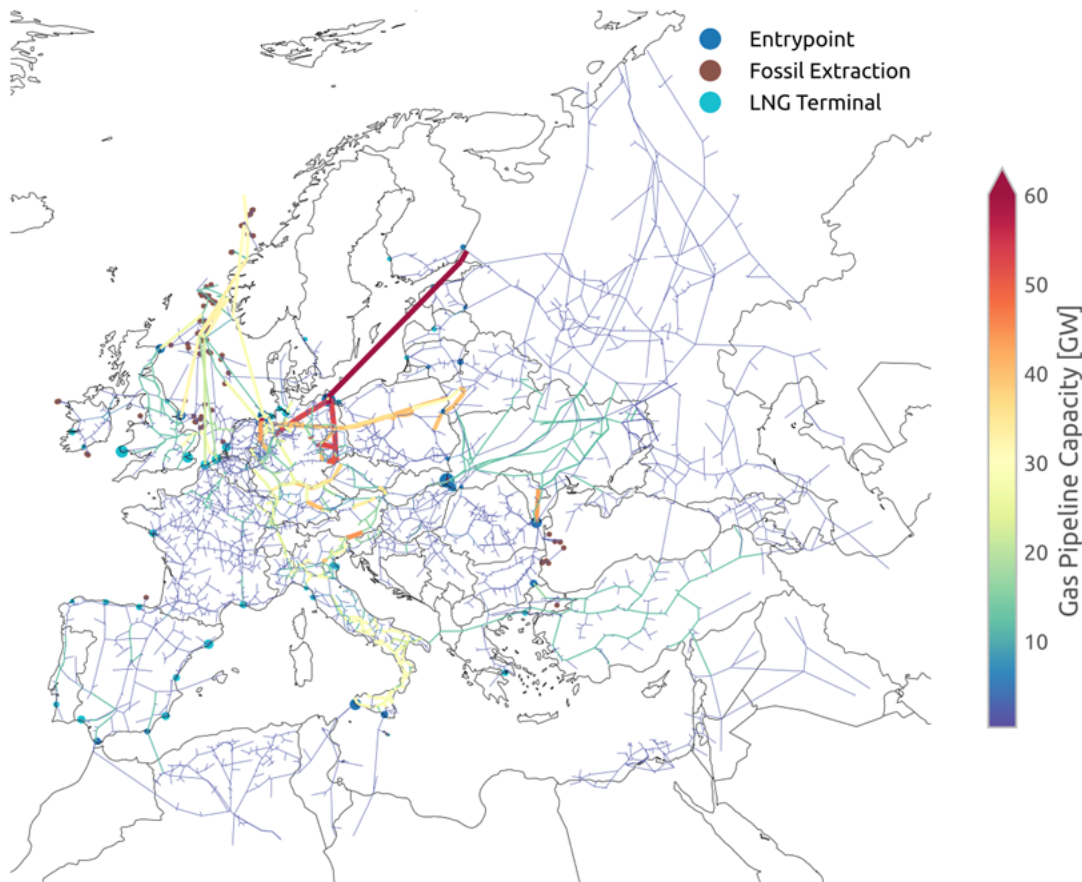
2.3.8 Biomass Supply

Biomass supply potentials for each European country are taken from the JRC ENSPRESO database where data is available for various years (2010, 2020, 2030, 2040 and 2050) and scenarios (low, medium, high). No biomass import from outside Europe is assumed. More information on the data set can be found here.

2.3.9 Biomass demand

Biomass supply potentials for every NUTS2 region are taken from the JRC ENSPRESO database where data is available for various years (2010, 2020, 2030, 2040 and 2050) and different availability scenarios (low, medium, high). No biomass import from outside Europe is assumed. More information on the data set can be found here. The data for NUTS2 regions is mapped to PyPSA-Eur-Sec model regions in proportion to the area overlap.

The desired scenario can be selected in the PyPSA-Eur-Sec configuration. The script for building the biomass potentials from the JRC ENSPRESO data base is located here. Consult the script to see the keywords that specify the scenario options.

The configuration also allows the user to define how the various types of biomass are used in the model by using the following categories: biogas, solid biomass, and not included. Feedstocks categorized as biogas, typically manure and sludge waste, are available to the model as biogas, which can be upgraded to biomethane. Feedstocks categorized as solid biomass, e.g. secondary forest residues or municipal waste, are available for combustion in combined-heat-and-power (CHP) plants and for medium temperature heat (below 500 °C) applications in industry. It can also converted to gas or liquid fuels.

Feedstocks labeled as not included are ignored by the model.

A typical use case for biomass would be the medium availability scenario for 2030 where only residues from agriculture and forestry as well as biodegradable municipal waste are considered as energy feedstocks. Fuel crops are avoided because they compete with scarce land for food production, while primary wood, as well as wood chips and pellets, are avoided because of concerns about sustainability. See the supporting materials of the paper for more details.

Solid biomass conversion and use

Solid biomass can be used directly to provide process heat up to 500C in the industry. It can also be burned in CHP plants and boilers associated with heating systems. These technologies are described elsewhere (see Large-scale CHP and *Industry demand*).

Solid biomass can be converted to syngas if the option is enabled in the config file. In this case the model will enable the technology BioSNG both with and without the option for carbon capture (see Technology-data repository).

Liquefaction of solid biomass can be enabled allowing the model to convert it into liquid hydrocarbons that can replace conventional oil products. This technology also comes with and without carbon capture (see Technology-data repository).

Transport of solid biomass

The transport of solid biomass can either be assumed unlimited between countries or it can be associated with a country specific cost per MWh/km. In the config file these options are toggled here. If the option is off, use of solid biomass is transport. If it is turned on, a biomass transport network will be created between all nodes. This network resembles road transport of biomass and the cost of transportation is a variable cost which is proportional to distance and a country specific cost per MWh/km. The latter is estimated from the country specific costs per ton/km used in the publication "The JRC-EU-TIMES model. Bioenergy potentials for EU and neighbouring countries".

Biogas transport and use

Biogas will be aggregated into a common European resources if a gas network is not modelled explicitly, i.e., the gas_network option is set to false. If, on the other hand, a gas network is included, the biogas potential will be associated with each node of origin. The model can only use biogas by first upgrading it to natural gas quality [see *Methane supply*] (bio methane) which is fed into the general gas network.

2.3.10 Oil-based products demand

Naphtha is used as a feedstock in the chemicals industry (see Chemicals Industry). Furthermore, kerosene is used as transport fuel in the aviation sector (see Aviation). Non-electrified agriculture machinery also consumes gasoline. Land transport [(see Land transport) that is not electrified or converted into using H_2-fuel cells also consumes oil-based products. While there is regional distribution of demand, the carrier is copperplated in the model, which means that transport costs and constraints are neglected.

2.3.11 Oil-based products supply

Oil-based products can be either of fossil origin or synthetically produced by combining H_2 (see *Hydrogen supply*) and captured CO_2 (see *Carbon dioxide capture, usage and sequestration (CCU/S)*) in Fischer-Tropsch plants

$$CO + (2 + 1)H_2 \text{ß} C_n H_{2n+2} + H_2 O$$
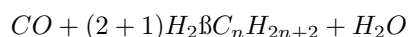
with costs as included from the technology-data repository. The waste heat from the Fischer-Tropsch process is supplied to district heating networks. The share of fossil and synthetic oil is an optimisation result depending on the techno-economic assumptions.

Oil-based transport

Liquid hydrocarbons are assumed to be transported freely among the model region since future demand is predicted to be low, transport costs for liquids are low and no bottlenecks are expected.

2.3.12 Industry demand

Industry demand is split into a dozen different sectors with specific energy demands, process emissions of carbon dioxide, as well as existing and prospective mitigation strategies.

The Subsection overview below provides a general description of the modelling approach for the industry sector. The following subsections describe the current energy demands, available mitigation strategies, and whether mitigation is exogenously fixed or co-optimised with the other components of the model for each industry subsector in more detail. See details for Iron and Steel (see Iron and Steel), Chemicals Industry and Ammonia (see Chemicals Industry), Non-metallic Mineral products , Non-ferrous Metals , and other Industry Subsectors.

Overview

Greenhouse gas emissions associated with industry can be classified into energy-related and process-related emissions. Today, fossil fuels are used for process heat energy in the chemicals industry, but also as a non-energy feedstock for chemicals like ammonia (NH_3), ethylene (C_2H_4) and methanol (CH_3OH). Energy-related emissions can be curbed by using low-emission energy sources. The only option to reduce process-related emissions is by using an alternative manufacturing process or by assuming a certain rate of recycling so that a lower amount of virgin material is needed.

The overarching modelling procedure can be described as follows. First, the energy demands and process emissions for every unit of material output are estimated based on data from the JRC-IDEES database and the fuel and process switching described in the subsequent sections. Second, the 2050 energy demands and process emissions are calculated using the per-unit-of-material ratios based on the industry transformations and the country-level material production in 2015, assuming constant material demand.

Missing or too coarsely aggregated data in the JRC-IDEES database is supplemented with additional datasets: Eurostat energy balances, United States, Geological Survey for ammonia production, DECHEMA for methanol and chlorine, and national statistics from Switzerland.

Where there are fossil and electrified alternatives for the same process (e.g. in glass manufacture or drying), we assume that the process is completely electrified. Current electricity demands (lighting, air compressors, motor drives, fans, pumps) will remain electric. Processes that require temperatures below 500 °C are supplied with solid biomass,

since we assume that residues and wastes are not suitable for high-temperature applications. We see solid biomass use primarily in the pulp and paper industry, where it is already widespread, and in food, beverages and tobacco, where it replaces natural gas. Industries which require high temperatures (above 500 °C), such as metals, chemicals and non-metallic minerals are either electrified where suitable processes already exist, or the heat is provided with synthetic methane.

Hydrogen for high-temperature process heat is not part of the model currently.

Where process heat is required, our approach depends on the necessary temperature. For example, due to the high share of high-temperature process heat demand (see Naegler et al. and Rehfeldt el al.), we disregard geothermal and solar thermal energy as sources for process heat since they cannot attain high-temperature heat.

The following figure shows the final consumption of energy and non-energy feedstocks in industry today in comparison to the scenario in 2050 assumed in Neumann et al.
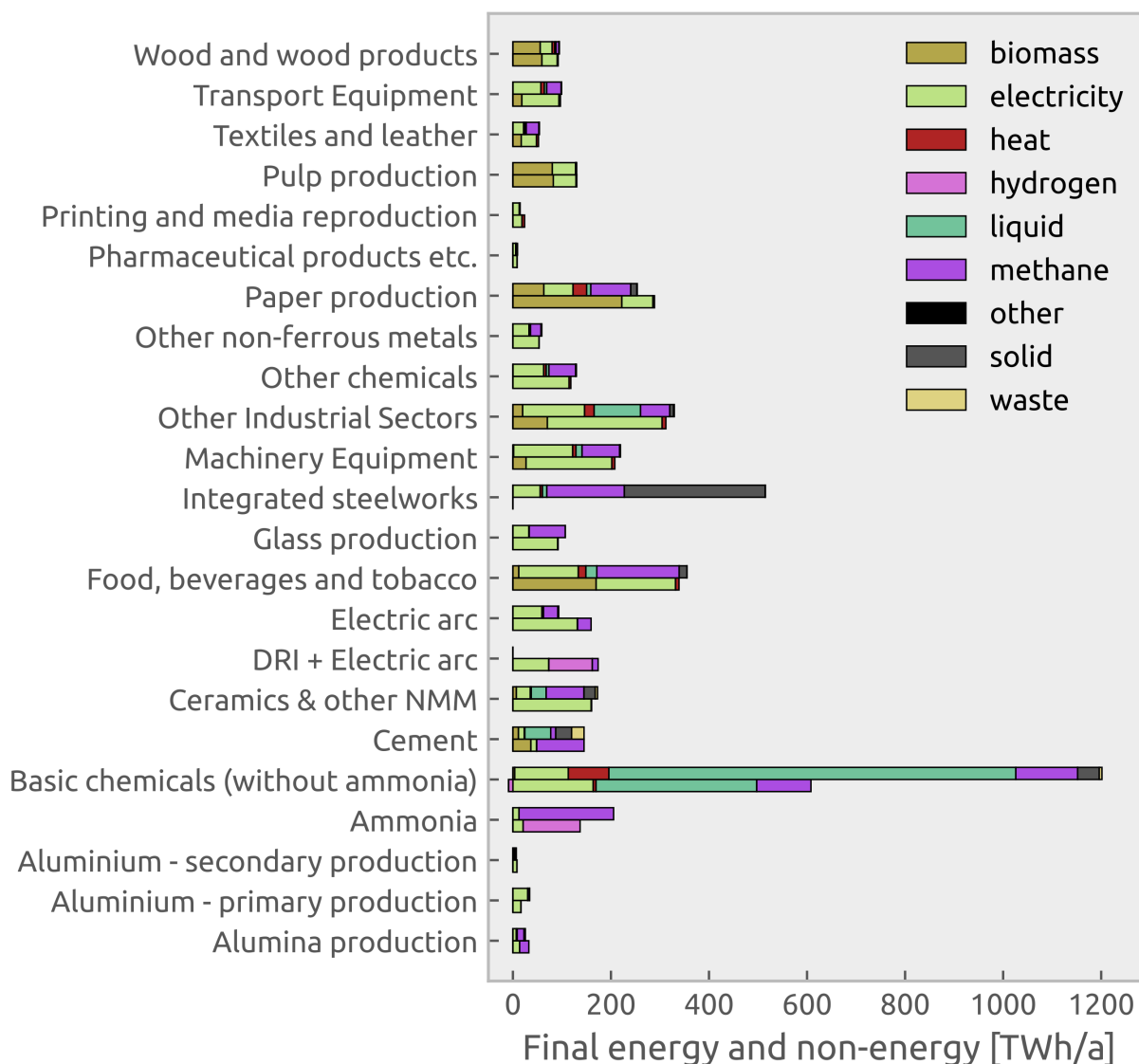
The following figure shows the process emissions in industry today (top bar) and in 2050 without carbon capture (bottom bar) assumed in Neumann et al.
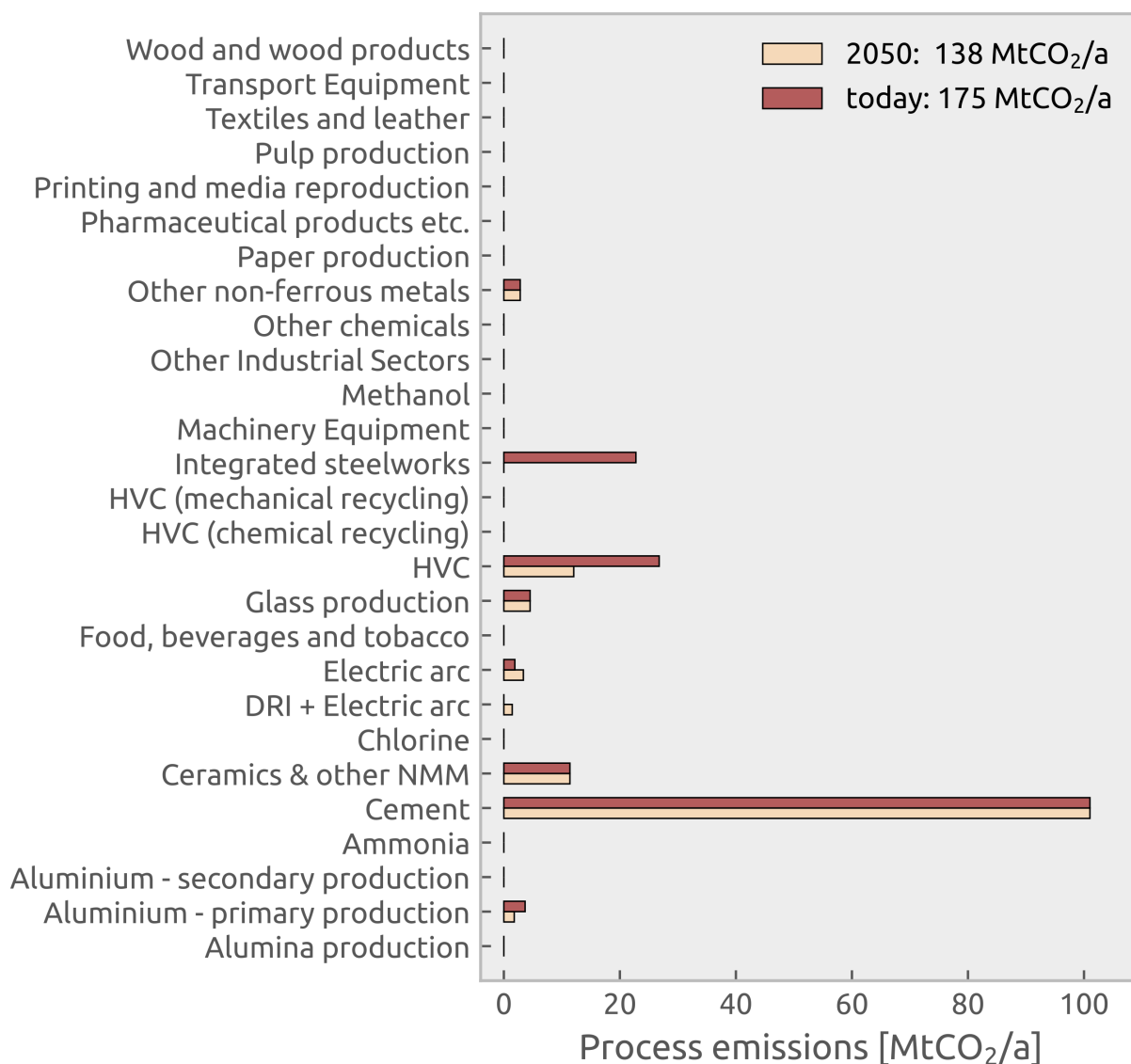
Inside each country the industrial demand is then distributed using the Hotmaps Industrial Database, which is illustrated in the figure below. This open database includes georeferenced industrial sites of energy-intensive industry sectors in EU28, including cement, basic chemicals, glass, iron and steel, non-ferrous metals, non-metallic minerals, paper, and refineries subsectors. The use of this spatial dataset enables the calculation of regional and process-specific energy demands. This approach assumes that there will be no significant migration of energy-intensive industries.
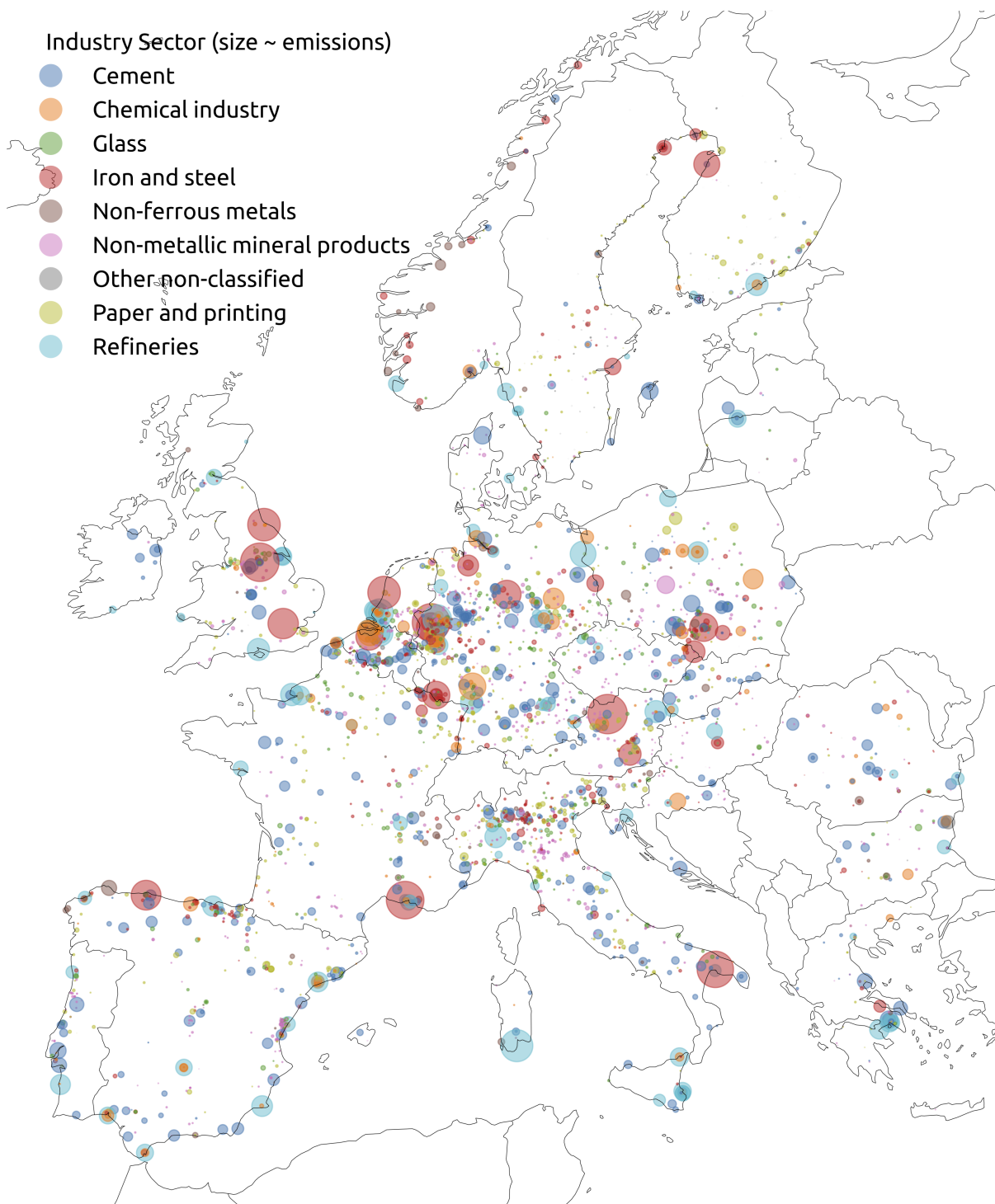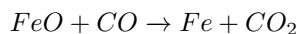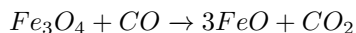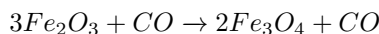
Iron and Steel

Two alternative routes are used today to manufacture steel in Europe. The primary route (integrated steelworks) represents 60% of steel production, while the secondary route (electric arc furnaces, EAF), represents the other 40% (Lechtenböhmer et. al).

The primary route uses blast furnaces in which coke is used to reduce iron ore into molten iron, which is then converted

into steel:

$$CO_2 + C \rightarrow 2CO$$

$$3Fe_2O_3 + CO \rightarrow 2Fe_3O_4 + CO$$

$$Fe_3O_4 + CO \rightarrow 3FeO + CO_2$$

$$FeO + CO \rightarrow Fe + CO_2$$

The primary route of steelmaking implies large process emissions of 0.22 t $_{CO_2}$ /t of steel, amounting to 7% of global greenhouse gas emissions (Vogl et. al).

In the secondary route, electric arc furnaces are used to melt scrap metal. This limits the CO_2 emissions to the burning of graphite electrodes (Friedrichsen et. al), and reduces process emissions to 0.03 t $_{CO_2}$ /t of steel.

We assume that the primary route can be replaced by a third route in 2050, using direct reduced iron (DRI) and subsequent processing in an EAF.

$$3Fe_2O_3 + H_2 \rightarrow 2Fe_3O_4 + H_2O$$

$$Fe_3O_4 + H_2 \rightarrow 3FeO + H_2O$$

$$FeO + H_2 \rightarrow Fe + H_2O$$
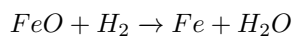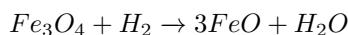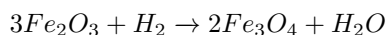
This circumvents the process emissions associated with the use of coke. For hydrogen- based DRI, we assume energy requirements of 1.7 MWh $_{H_2}$ /t steel (Vogl et. al) and 0.322 MWh $_{el}$/t steel (HYBRIT 2016).

The share of steel produced via the primary route is exogenously set in the config file. The share of steel obtained via hydrogen-based DRI plus EAF is also set exogenously in the config file. The remaining share is manufactured through the secondary route using scrap metal in EAF. Bioenergy as alternative to coke in blast furnaces is not considered in the model (Mandova et.al, Suopajärvi et.al).

For the remaining subprocesses in this sector, the following transformations are assumed. Methane is used as energy source for the smelting process. Activities associated with furnaces, refining and rolling, and product finishing are electrified assuming the current efficiency values for these cases. These transformations result in changes in process emissions as outlined in the process emissions figure presented in the industry overview section (see Overview).

Chemicals Industry

The chemicals industry includes a wide range of diverse industries, including the production of basic organic compounds (olefins, alcohols, aromatics), basic inorganic compounds (ammonia, chlorine), polymers (plastics), and end-user products (cosmetics, pharmaceutics).

The chemicals industry consumes large amounts of fossil-fuel based feedstocks (see Levi et. al), which can also be produced from renewables as outlined for hydrogen (see *Hydrogen supply*), for methane (see *Methane supply*), and for oil-based products (see *Oil-based products supply*). The ratio between synthetic and fossil-based fuels used in the industry is an endogenous result of the optimisation.

The basic chemicals consumption data from the JRC IDEES database comprises high- value chemicals (ethylene, propylene and BTX), chlorine, methanol and ammonia. However, it is necessary to separate out these chemicals because their current and future production routes are different.

Statistics for the production of ammonia, which is commonly used as a fertilizer, are taken from the USGS for every country. Ammonia can be made from hydrogen and nitrogen using the Haber-Bosch process.

$$N_2 + 3H_2 \rightarrow 2NH_3$$
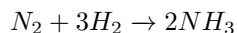
The Haber-Bosch process is not explicitly represented in the model, such that demand for ammonia enters the model as a demand for hydrogen (6.5 MWh $_{H_2}$ / t $_{NH_3}$) and electricity (1.17 MWh $_{el}$ /t $_{NH_3}$) (see Wang et. al). Today,

natural gas dominates in Europe as the source for the hydrogen used in the Haber-Bosch process, but the model can choose among the various hydrogen supply options described in the hydrogen section (see *Hydrogen supply*)

The total production and specific energy consumption of chlorine and methanol is taken from a DECHEMA report. According to this source, the production of chlorine amounts to 9.58 MtCl/a, which is assumed to require electricity at 3.6 MWh $_{el}$/t of chlorine and yield hydrogen at 0.937 MWh $_{H_2}$/t of chlorine in the chloralkali process. The production of methanol adds up to 1.5 MtMeOH/a, requiring electricity at 0.167 MWh $_{el}$/t of methanol and methane at 10.25 MWh $_{CH_4}$/t of methanol.

The production of ammonia, methanol, and chlorine production is deducted from the JRC IDEES basic chemicals, leaving the production totals of high-value chemicals. For this, we assume that the liquid hydrocarbon feedstock comes from synthetic or fossil- origin naphtha (14 MWh $_{naphtha}$/t of HVC, similar to Lechtenböhmer et al), ignoring the methanol-to-olefin route. Furthermore, we assume the following transformations of the energy-consuming processes in the production of plastics: the final energy consumption in steam processing is converted to methane since requires temperature above 500 °C (4.1 MWh $_{CH_4}$ /t of HVC, see Rehfeldt et al.); and the remaining processes are electrified using the current efficiency of microwave for high-enthalpy heat processing, electric furnaces, electric process cooling and electric generic processes (2.85 MWh $_{el}$/t of HVC).

The process emissions from feedstock in the chemical industry are as high as 0.369 t $_{CO_2}$/t of ethylene equivalent. We consider process emissions for all the material output, which is a conservative approach since it assumes that all plastic-embedded CO_2 will eventually be released into the atmosphere. However, plastic disposal in landfilling will avoid, or at least delay, associated CO_2 emissions.

Circular economy practices drastically reduce the amount of primary feedstock needed for the production of plastics in the model (see Kullmann et al., Meys et al. (2021), Meys et al. (2020), Gu et al.) and consequently, also the energy demands and level of process emission. The percentage of plastics that are assumed to be mechanically recycled can be selected in the config file, as well as the percentage that is chemically recycled, see config file The energy consumption for those recycling processes are respectively 0.547 MWh $_{el}$/t of HVC (as indicated in the config file) (Meys et al. (2020)), and 6.9 MWh $_{el}$/t of HVC (as indicated in the config file) based on pyrolysis and electric steam cracking (see Materials Economics report).

Non-metallic Mineral Products

This subsector includes the manufacturing of cement, ceramics, and glass.

Cement

Cement is used in construction to make concrete. The production of cement involves high energy consumption and large process emissions. The calcination of limestone to chemically reactive calcium oxide, also known as lime, involves process emissions of 0.54 t $_{CO_2}$ /t cement (see Akhtar et al..

$$CaCO_3 \rightarrow CaO + CO_2$$

Additionally, CO_2 is emitted from the combustion of fossil fuels to provide process heat. Thereby, cement constitutes the biggest source of industry process emissions in Europe.

Cement process emissions can be captured assuming a capture rate of 90%. Whether emissions are captured is decided by the model taking into account the capital costs of carbon capture modules. The electricity and heat demand of process emission carbon capture is currently ignored. For net-zero emission scenarios, the remaining process emissions need to be compensated by negative emissions.

With the exception of electricity demand and biomass demand for low-temperature heat (0.06 MWh/t and 0.2 MWh/t), the final energy consumption of this subsector is assumed to be supplied by methane (0.52 MWh/t), which is capable of delivering the required high-temperature heat. This implies a switch from burning solid fuels to burning gas which will require adjustments of the kilns. The share of fossil vs. synthetic methane consumed is a result of the optimisation

Ceramics

The ceramics sector is assumed to be fully electrified based on the current efficiency of already electrified processes which include microwave drying and sintering of raw materials, electric kilns for primary production processes, electric furnaces for the product finishing. In total, the final electricity consumption is 0.44 MWh/t of ceramic. The

manufacturing of ceramics includes process emissions of 0.03 t $_{CO_2}$/t of ceramic. For a detailed overview of the ceramics industry sector see Furszyfer Del Rio et al.

Glass

The production of glass is assumed to be fully electrified based on the current efficiency of electric melting tanks and electric annealing which adds up to an electricity demand of 2.07 MWh $_{el}$/t of glass. The manufacturing of glass incurs process emissions of 0.1 t $_{CO_2}$/t of glass. Potential efficiency improvements, which according to Lechtenböhmer et al could reduce energy demands to 0.85 MW $_{el}$/t of glass, have not been considered. For a detailed overview of the glass industry sector see Furszyfer Del Rio et al.

Non-ferrous Metals

The non-ferrous metal subsector includes the manufacturing of base metals (aluminium, copper, lead, zink), precious metals (gold, silver), and technology metals (molybdenum, cobalt, silicon).

The manufacturing of aluminium accounts for more than half of the final energy consumption of this subsector. Two alternative processing routes are used today to manufacture aluminium in Europe. The primary route represents 40% of the aluminium pro- duction, while the secondary route represents the remaining 60%.

The primary route involves two energy-intensive processes: the production of alumina from bauxite (aluminium ore) and the electrolysis to transform alumina into aluminium via the Hall-Héroult process

$$2Al_2O_3 + 3C \rightarrow 4Al + 3CO_2$$
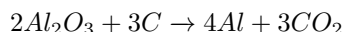
The primary route requires high-enthalpy heat (2.3 MWh/t) to produce alumina which is supplied by methane and causes process emissions of 1.5 t $_{CO_2}$/t aluminium. According to Friedrichsen et al., inert anodes might become commercially available by 2030 that would eliminate the process emissions, but they are not included in the model. Assuming all subprocesses are electrified, the primary route requires 15.4 MWh $_{el}$/t of aluminium.

In the secondary route, scrap aluminium is remelted. The energy demand for this process is only 10% of the primary route and there are no associated process emissions. Assuming all subprocesses are electrified, the secondary route requires 1.7 MWh/t of aluminium. The share of aliminum manufactured by the primary and secondary route can be selected in the config file]

For the other non-ferrous metals, we assume the electrification of the entire manufacturing process with an average electricity demand of 3.2 MWh $_{el}$/t lead equivalent.

Other Industry Subsectors

The remaining industry subsectors include (a) pulp, paper, printing, (b) food, beverages, tobacco, (c) textiles and leather, (d) machinery equipment, (e) transport equipment, (f) wood and wood products, (g) others. Low- and mid-temperature process heat in these industries is assumed to be supplied by biomass while the remaining processes are electrified. None of the subsectors involve process emissions.

2.3.13 Agriculture demand

Energy demands for the agriculture, forestry and fishing sector per country are taken from the JRC-IDEES database. Missing countries are filled with Eurostat data. Agricultural energy demands are split into electricity (lighting, ventilation, specific electricity uses, electric pumping devices), heat (specific heat uses, low enthalpy heat), and machinery oil (motor drives, farming machine drives, diesel-fueled pumping devices). Heat demand is assigned at "services rural heat" buses. Time series for demands are assumed to be constant and distributed inside countries by population.

2.3.14 Transportation

Annual energy demands for land transport, aviation and shipping for every country are retrieved from JRC-IDEES data set. Below, the details of how each of these categories are treated is explained.

Land transport

Both road and rail transport is combined as land transport demand although electrified rail transport is excluded because that demand is included in the current electricity demand.

The most important settings for land transport are the exogenously fixed fuel mix (an option enabling the endogeous optimization of transport electrification is planned but not yet implemented). In the config file, the share of battery electric vehicles (BEV) and hydrogen fuel cell vehicles (FCEV) can be set. The remaining percentage will be treated as internal combustion engines (ICE) that consume oil products.

Battery Electric vehicles (BEV)

For the electrified land transport, country-specific factors are computed by comparing the current car final energy consumption per km in (average for Europe 0.7 kWh/km) to the 0.18 kWh/km value assumed for battery-to-wheels efficiency in EVs. The characteristic weekly profile provided by the German Federal Highway Research Institute (BASt) is used to obtain hourly time series for European countries taking into account the corresponding local times. Furthermore, a temperature dependence is included in the time series to account for heating/cooling demand in transport. For temperatures below/above certain threshold values, e.g. 15 °C/20 °C, temperature coefficients of typically 0.98%/°C and 0.63%/°C are assumed, based on the paper.

For BEVs the user can define the storage energy capacity, charging power capacity, and charging efficiency.

For BEV, smart charging is an option. A certain share of the BEV fleet can shift their charging time. The BEV state of charge is forced to be higher than a set percentage, e.g. 75%, every day at a specified hour, e.g., 7 am, to ensure that the batteries are sufficiently charged for peak usage in the morning and they not behave as seasonal storage. They also have the option to participate in vehicle-to-grid (V2G) services to facilitate system operation if that is enabled.

The battery cost of BEV is not included in the model since it is assumed that BEV owners buy them to primarily satisfy their mobility needs.

Hydrogen fuel cell vehicles (FCEV)

The share of all land transport that is specified to be be FCEV will be converted to a demand for hydrogen (see *Hydrogen supply*) using the FCEV efficiency.

FCEVs are typically used to simulate demand for transport that is hard to electrify directly, e.g. heavy construction machinery. But it may also be used to investigate a more widespread adoption of the technology.

Internal combustion engine vehicles (ICE)

All land transport that is not specified to be either BEV or FCEV will be treated as conventional ICEs. The transport demand is converted to a demand for oil products (see *Oil-based products supply*) using the ICE efficiency.

Aviation

The demand for aviation includes international and domestic use. It is modelled as an oil demand since aviation consumes kerosene. This can be produced synthetically or have fossil-origin (see *Oil-based products supply*).

Shipping

Shipping energy demand is covered by a combination of oil and hydrogen. Other fuel options, like methanol or ammonia, are currently not included in PyPSA-Eur-Sec. The share of shipping that is assumed to be supplied by hydrogen can be selected in the config file.

To estimate the hydrogen demand, the average fuel efficiency of the fleet is used in combination with the efficiency of the fuel cell defined in the technology-data repository. The average fuel efficiency is set in the config file.

The consumed hydrogen comes from the general hydrogen bus where it can be produced by SMR, SMR+CC or electrolysers (see *Hydrogen supply*). The fraction that is not converted into hydrogen use oil products, i.e. is connected to the general oil bus.

The energy demand for liquefaction of the hydrogen used for shipping can be included. If this option is selected, liquifaction will happen at the node where the shipping demand occurs.

2.3.15 Carbon dioxide capture, usage and sequestration (CCU/S)

PyPSA-Eur-Sec includes carbon capture from air (i.e., direct air capture (DAC)), electricity generators, and industrial facilities. It furthermore includes carbon dioxide storage and transport, the usage of carbon dioxide in synthetic methane and oil products, as well as the sequestration of carbon dioxide underground.

Carbon dioxide capture

For the following point source emissions, carbon capture is applicable:

- Industry process emissions, e.g., from limestone in cement production

- Methane or biomass used for process heat in the industry

- Hydrogen production by SMR

- CHP plants using biomass or methane

- Coal power plants.

Point source emissions are captured assuming a capture rate, e.g. 90%, which can be specified in the config file. The electricity and heat demand of process emission carbon capture is currently ignored.

DAC (if included) includes the adsorption phase where electricity and heat consumptionsare required to assist the adsorption process and regenerate the adsorbent. It also includes the drying and compression of CO_2 prior to storage which consumes electricity and rejects heat.

Carbon dioxide usage

Captured CO_2 can be used to produce synthetic methane and synthetic oil products (e.g. naphtha). If captured carbon is used, the CO_2 emissions of the synthetic fuels are net-neutral.

Carbon dioxide sequestration

Captured CO_2 can also be sequestered underground up to an annual sequestration limit of 200 Mt $_{CO_2}$/a. This limit can be chosen in the config file. As stored carbon dioxide is modelled as a single node for Europe, CO_2 transport constraints are neglected. Since CO_2 sequestration is an immature technology, the cost assumption is defined in the config file.

Carbon dioxide transport

Carbon dioxide can be modelled as a single node for Europe (in this case, CO_2 transport constraints are neglected). A network for modelling the transport of CO_2 among the different nodes can also be created if selected in the config file.

2.4 Technology and cost assumptions

Techno-Economic Assumptions

For the technological assumptions (cost, efficiency, lifetime, etc.), we take estimates for the investment year specified in the config. Many of those come from a database published by the Danish Energy Agency (DEA). Assumptions are maintained at the technology data repository.

Foresight options

- *Overnight (greenfield) scenarios*

- *Myopic transition path*

- *Perfect foresight scenarios*

2.5 Overnight (greenfield) scenarios

The default is to calculate a rebuilding of the energy system to meet demand, a so-called overnight or greenfield approach.

For this, use `foresight : 'overnight'` in `config.yaml`, like the example in `config.default.yaml`.

In this case, the `planning_horizons : [2030]` scenario parameter can be set to use the year from which cost and other technology assumptions are set (forecasts for 2030 in this case).

2.6 Myopic transition path

The myopic code can be used to investigate progressive changes in a network, for instance, those taking place throughout a transition path. The capacities installed in a certain time step are maintained in the network until their operational lifetime expires.

The myopic approach was initially developed and used in the paper Early decarbonisation of the European Energy system pays off (2020) and later further extended in Speed of technological transformations required in Europe to achieve different climate goals (2022). The current implementation complies with the PyPSA-Eur-Sec standard working flow and is compatible with using the higher resolution electricity transmission model PyPSA-Eur rather than a one-node-per-country model.

The current code applies the myopic approach to generators, storage technologies and links in the power sector. It furthermore applies it to the space and water heating sector (e.g., the share of district heating and reduced space heat demand), industry processes (e.g., steel, direct reduced iron, and aluminum production via primary route), the share of fuel cell and battery electric vehicles in land transport, and the hydrogen share in shipping (see *Supply and demand* for further information).

The following subjects within the land transport and biomass currently do not evolve with the myopic approach:

- The percentage of electric vehicles that allow demand-side management and vehicle-to-grid services.

- The annual biomass potential (default year and scenario for which potential is taken is 2030, defined here)

2.6.1 Configuration

PyPSA-Eur-Sec has several configuration options which are collected in a config.yaml file located in the root directory. For myopic optimization, users should copy the provided default configuration `config.default.yaml` and make their own modifications and assumptions in the user-specific configuration file (`config.yaml`).

The following options included in the config.yaml file are relevant for the myopic code.

To activate the myopic option select `foresight: 'myopic'` in `config.yaml`.

The {planning_horizons} wildcard indicates the year in which the network is optimized. For a myopic optimization, this is equivalent to the investment year. To set the investment years which are sequentially simulated for the myopic investment planning, select for example:

planning_horizons:

- 2020

- 2030

- 2040

- 2050

in `config.yaml`.

existing capacities

Grouping years indicates the bins limits for grouping the existing capacities of different technologies. Note that separate bins are defined for the power and heating plants due to different data sources.

`grouping_years_power:` `[1980, 1985, 1990, 1995, 2000, 2005, 2010, 2015, 2020, 2025, 2030]`

`grouping_years_heat:` `[1980, 1985, 1990, 1995, 2000, 2005, 2010, 2015, 2019]`

threshold capacity

If for a technology, node, and grouping bin, the capacity is lower than threshold_capacity, it is ignored.

`threshold_capacity:` `10`

conventional carriers

Conventional carriers indicate carriers used in the existing conventional technologies.

conventional_carriers:

- lignite

- coal

- oil

- uranium

2.6.2 Options

The total carbon budget for the entire transition path can be indicated in the sector_opts in `config.yaml`. The carbon budget can be split among the `planning_horizons` following an exponential or beta decay. E.g. `'cb40ex0'` splits a carbon budget equal to 40 Gt $_{CO_2}$ following an exponential decay whose initial linear growth rate r is zero. They can also follow some user-specified path, if defined here. The paper Speed of technological transformations required in Europe to achieve different climate goals (2022) defines CO_2 budgets corresponding to global temperature increases (1.5C – 2C) as response to the emissions. Here, global carbon budgets are converted to European budgets assuming equal-per capita distribution which translates into a 6.43% share for Europe. The carbon budgets are in this paper distributed throughout the transition paths assuming an exponential decay. Emissions e(t) in every year t are limited by

$$e(t) = e_0(1 + (r + m)t)e^{-mt}$$

where r is the initial linear growth rate, which here is assumed to be r=0, and the decay parameter m is determined by imposing the integral of the path to be equal to the budget for Europe. Following this approach, the CO_2 budget is defined. Following the same approach as in this paper, add the following to the `scenario.sector_opts` E.g. `-cb25.7ex0` (1.5C increase) Or `cb73.9ex0` (2C increase). See details in Supplemental Note S1 Speed of technological transformations required in Europe to achieve different climate goals (2022).

2.6.3 General myopic code structure

The myopic code solves the network for the time steps included in `planning_horizons` in a recursive loop, so that:

1. The existing capacities (those installed before the base year are added as fixed capacities with p_nom=value, p_nom_extendable=False). E.g. for baseyear=2020, capacities installed before 2020 are added. In addition, the network comprises additional generator, storage, and link capacities with p_nom_extendable=True. The non-solved

network is saved in `results/run_name/networks/prenetworks-brownfield`. The base year is the first element in `planning_horizons`. Step 1 is implemented with the rule add_baseyear for the base year and with the rule add_brownfield for the remaining planning_horizons.

2. The 2020 network is optimized. The solved network is saved in `results/run_name/networks/postnetworks`

3. For the next planning horizon, e.g. 2030, the capacities from a previous time step are added if they are still in operation (i.e., if they fulfil planning horizon <= commissioned year + lifetime). In addition, the network comprises additional generator, storage, and link capacities with p_nom_extendable=True. The non-solved network is saved in `results/run_name/networks/prenetworks-brownfield`.

Steps 2 and 3 are solved recursively for all the planning_horizons included in `config.yaml`.

2.6.4 Rule overview

- rule add_existing baseyear

  The rule add_existing_baseyear loads the network in 'results/run_name/networks/prenetworks' and performs the following operations:

  1. Add the conventional, wind and solar power generators that were installed before the base year.

  2. Add the heating capacities that were installed before the base year.

  The existing conventional generators are retrieved from the powerplants.csv file generated by pypsa-eur which, in turn, is based on the powerplantmatching database.

  Existing wind and solar capacities are retrieved from IRENA annual statistics and distributed among the nodes in a country proportional to capacity factor. (This will be updated to include capacity distributions closer to reality.)

  Existing heating capacities are retrieved from the report Mapping and analyses of the current and future (2020 - 2030) heating/cooling fuel deployment (fossil/renewables).

  The heating capacities are assumed to have a lifetime indicated by the parameter lifetime in the configuration file, e.g 25 years. They are assumed to be decommissioned linearly starting on the base year, e.g., from 2020 to 2045.

  Then, the resulting network is saved in `results/run_name/networks/prenetworks-brownfield`.

- rule add_brownfield

  The rule add_brownfield loads the network in `results/run_name/networks/prenetworks` and performs the following operation:

  1. Read the capacities optimized in the previous time step and add them to the network if they are still in operation (i.e., if they fulfill planning horizon < commissioned year + lifetime)

  Then, the resulting network is saved in `results/run_name/networks/prenetworks_brownfield`.

2.7 Perfect foresight scenarios

Perfect foresight is currently under development but it is not yet implemented.

For this, use `foresight :  'perfect'` in `config.yaml`.

References

- *Release Notes*

- *Limitations*

2.8 Release Notes

2.8.1 Future release

Note: This unreleased version currently may require the master branches of PyPSA, PyPSA-Eur, and the technology-data repository.

- new feature

2.8.2 PyPSA-Eur-Sec 0.7.0 (16th February 2023)

This release includes many new features. Highlights include new gas infrastructure data with retrofitting options for hydrogen transport, improved carbon management and infrastructure planning, regionalised potentials for hydrogen underground storage and carbon sequestration, new applications for biomass, and explicit modelling of methanol and ammonia as separate energy carriers.

This release is known to work with PyPSA-Eur Version 0.7.0 and Technology Data Version 0.5.0.

Gas Transmission Network

- New rule `retrieve_gas_infrastructure_data` that downloads and extracts the SciGRID_gas IG-GIELGN dataset from zenodo. It includes data on the transmission routes, pipe diameters, capacities, pressure, and whether the pipeline is bidirectional and carries H-Gas or L-Gas.

- New rule `build_gas_network` processes and cleans the pipeline data from SciGRID_gas. Missing or uncertain pipeline capacities can be inferred by diameter.

- New rule `build_gas_input_locations` compiles the LNG import capacities (from the Global Energy Monitor's Europe Gas Tracker, pipeline entry capacities and local production capacities for each region of the model. These are the regions where fossil gas can eventually enter the model.

- New rule `cluster_gas_network` that clusters the gas transmission network data to the model resolution. Cross-regional pipeline capacities are aggregated (while pressure and diameter compatibility is ignored), intra-regional pipelines are dropped. Lengths are recalculated based on the regions' centroids.

- With the option `sector: gas_network:`, the existing gas network is added with a lossless transport model. A length-weighted k-edge augmentation algorithm can be run to add new candidate gas pipelines such that all regions of the model can be connected to the gas network. The number of candidates can be controlled via the setting `sector: gas_network_connectivity_upgrade:`. When the gas network is activated, all the gas demands are regionally disaggregated as well.

- New constraint allows endogenous retrofitting of gas pipelines to hydrogen pipelines. This option is activated via the setting `sector: H2_retrofit:`. For every unit of gas pipeline capacity dismantled, `sector: H2_retrofit_capacity_per_CH4` units are made available as hydrogen pipeline capacity in the corresponding corridor. These repurposed hydrogen pipelines have lower costs than new hydrogen pipelines. Both new and repurposed pipelines can be built simultaneously. The retrofitting option `sector: H2_retrofit:` also works with a copperplated methane infrastructure, i.e. when `sector: gas_network: false`.

- New hydrogen pipelines can now be built where there are already power or gas transmission routes. Previously, only the electricity transmission routes were considered.

Carbon Management and Biomass

- Add option to spatially resolve carrier representing stored carbon dioxide (`co2_spatial`). This allows for more detailed modelling of CCUTS, e.g. regarding the capturing of industrial process emissions, usage as feedstock for electrofuels, transport of carbon dioxide, and geological sequestration sites.

- Add option for regionally-resolved geological carbon dioxide sequestration potentials through new rule `build_sequestration_potentials` based on [CO2StoP](). This can be controlled in the section `regional_co2_sequestration_potential` of the `config.yaml`. It includes options to select the level of conservatism, whether onshore potentials should be included, the respective upper and lower limits per region, and an annualisation parameter for the cumulative potential. The defaults are preliminary and will be validated the next release.

- Add option to sweep the global CO2 sequestration potentials with keyword `seq200` in the `{sector_opts}` wildcard (for limit of 200 Mt CO2).

- Add option to include [Allam cycle gas power plants]() (`allam_cycle`).

- Add option for planning a new carbon dioxide network (`co2network`).

- Separate option to regionally resolve biomass (`biomass_spatial`) from option to allow biomass transport (`biomass_transport`).

- Add option for biomass boilers (wood pellets) for decentral heating.

- Add option for BioSNG (methane from biomass) with and without carbon capture.

- Add option for BtL (biomass to liquid fuel/oil) with and without carbon capture.

Other new features

- Add regionalised hydrogen salt cavern storage potentials from [Technical Potential of Salt Caverns for Hydrogen Storage in Europe](). This data is compiled in a new rule `build_salt_cavern_potentials`.

- Add option to resolve ammonia as separate energy carrier with Haber-Bosch synthesis, ammonia cracking, storage and industrial demand. The ammonia carrier can be nodally resolved or copperplated across Europe (see `ammonia`).

- Add methanol as energy carrier, methanolisation as process, and option for methanol demand in shipping sector.

- Shipping demand now defaults to methanol rather than liquefied hydrogen until 2050.

- Demand for liquid hydrogen in international shipping is now geographically distributed by port trade volumes in a new rule `build_shipping_demand` using data from the [World Bank Data Catalogue](). Domestic shipping remains distributed by population.

- Add option to aggregate network temporally using representative snapshots or segments (with [tsam]()).

- Add option for minimum part load for Fischer-Tropsch plants (default: 90%) and methanolisation plants (default: 50%).

- Add option to use waste heat of electrolysis in district heating networks (`use_electrolysis_waste_heat`).

- Add option for coal CHPs with carbon capture (see `coal_cc`).

- In overnight optimisation, it is now possible to specify a year for the technology cost projections separate from the planning horizon.

- New config options for changing energy demands in aviation (`aviation_demand_factor`) and HVC industry (`HVC_demand_factor`), as well as explicit ICE shares for land transport (`land_transport_ice_share`) and agriculture machinery (`agriculture_machinery_oil_share`).

- It is now possible to merge residential and services heat buses to reduce the problem size (see `cluster_heat_nodes`).

- Added option to tweak (almost) any configuration parameter through the `{sector_opts}` wildcard. The regional_co2_sequestration_potential is triggered by the prefix `CF+` after which it is possible to pipe to any setting that does not contain underscores (_). Example: `CF+sector+v2g+false` disables vehicle-to-grid flexibility.

- Option `retrieve_sector_databundle` to automatically retrieve and extract data bundle.

- Removed the need to clone `technology-data` repository in a parallel directory. The new approach automatically retrieves the technology data from remote in the rule `retrieve_cost_data`.

- Improved network plots including better legends, hydrogen retrofitting network display, and change to EqualEarth projection. A new color scheme for technologies was also introduced.

- Add two new rules `build_transport_demand` and `build_population_weighted_energy_totals` using code previously contained in `prepare_sector_network`.

- Rules that convert weather data with `atlite` now largely run separately for categories residential, rural and total.

- Units are assigned to the buses. These only provide a better understanding. The specifications of the units are not taken into account in the optimisation, which means that no automatic conversion of units takes place.

- Configuration file and wildcards are now stored under `n.meta` in every PyPSA network.

- Updated data bundle that includes the hydrogan salt cavern storage potentials.

- Updated and extended documentation in <https://pypsa-eur-sec.readthedocs.io/en/latest/>

- Added new rule `copy_conda_env` that exports a list of packages with which the workflow was executed.

- Add basic continuous integration using Github Actions.

- Add basic `rsync` setup.

Bugfixes

- The CO2 sequestration limit implemented as GlobalConstraint (introduced in the previous version) caused a failure to read in the shadow prices of other global constraints.

- Correct capital cost of Fischer-Tropsch according to new units in `technology-data` repository.

- Fix unit conversion error for thermal energy storage.

- For myopic pathway optimisation, set optimised capacities of power grid expansion of previous iteration as minimum capacity for next iteration.

- Further rather minor bugfixes for myopic optimisation code (see #256).

Many thanks to all who contributed to this release!

2.8.3 PyPSA-Eur-Sec 0.6.0 (4 October 2021)

This release includes improvements regarding the basic chemical production, the addition of plastics recycling, the addition of the agriculture, forestry and fishing sector, more regionally resolved biomass potentials, CO2 pipeline transport and storage, and more options in setting exogenous transition paths, besides many performance improvements.

This release is known to work with PyPSA-Eur Version 0.4.0, Technology Data Version 0.3.0 and PyPSA Version 0.18.0.

Please note that the data bundle has also been updated.

General

- With this release, we change the license from copyleft GPLv3 to the more liberal MIT license with the consent of all contributors.

New features and functionality

- Distinguish costs for home battery storage and inverter from utility-scale battery costs.

- Separate basic chemicals into HVC (high-value chemicals), chlorine, methanol and ammonia [#166].

- Add option to specify reuse, primary production, and mechanical and chemical recycling fraction of platics [#166].

- Include energy demands and CO2 emissions for the agriculture, forestry and fishing sector. It is included by default through the option A in the `sector_opts` wildcard. Part of the emissions (1.A.4.c) was previously assigned to "industry non-elec" in the `co2_totals.csv`. Hence, excluding the agriculture sector will now lead to a tighter CO2 limit. Energy demands are taken from the JRC IDEES database (missing countries filled with eurostat data) and are split into electricity (lighting, ventilation, specific electricity uses, pumping devices (electric)), heat (specific heat uses, low enthalpy heat) machinery oil (motor drives, farming machine drives, pumping devices (diesel)). Heat demand is assigned at "services rural heat" buses. Electricity demands are added to low-voltage buses. Time series for demands are constant and distributed inside countries by population [#147].

- Include today's district heating shares in myopic optimisation and add option to specify exogenous path for district heating share increase under `sector: district_heating:` [#149].

- Added option for hydrogen liquefaction costs for hydrogen demand in shipping. This introduces a new H2 liquid bus at each location. It is activated via `sector: shipping_hydrogen_liquefaction: true`.

- The share of shipping transformed into hydrogen fuel cell can be now defined for different years in the `config.yaml` file. The carbon emission from the remaining share is treated as a negative load on the atmospheric carbon dioxide bus, just like aviation and land transport emissions.

- The transformation of the Steel and Aluminium production can be now defined for different years in the `config.yaml` file.

- Include the option to alter the maximum energy capacity of a store via the `carrier+factor` in the `{sector_opts}` wildcard. This can be useful for sensitivity analyses. Example: `co2 stored+e2` multiplies the `e_nom_max` by factor 2. In this example, `e_nom_max` represents the CO2 sequestration potential in Europe.

- Use JRC ENSPRESO database to spatially disaggregate biomass potentials to PyPSA-Eur regions based on overlaps with NUTS2 regions from ENSPRESO (proportional to area) (#151).

- Add option to regionally disaggregate biomass potential to individual nodes (previously given per country, then distributed by population density within) and allow the transport of solid biomass. The transport costs are determined based on the JRC-EU-Times Bioenergy report in the new optional rule `build_biomass_transport_costs`. Biomass transport can be activated with the setting `sector: biomass_transport: true`.

- Add option to regionally resolve CO2 storage and add CO2 pipeline transport because geological storage potential, CO2 utilisation sites and CO2 capture sites may be separated. The CO2 network is built from zero based on the topology of the electricity grid (greenfield). Pipelines are assumed to be bidirectional and lossless. Furthermore, neither retrofitting of natural gas pipelines (required pressures are too high, 80-160 bar vs <80 bar) nor other modes of CO2 transport (by ship, road or rail) are considered. The regional representation of CO2 is activated with the config setting `sector: co2_network: true` but is deactivated by default. The global limit for CO2 sequestration now applies to the sum of all CO2 stores via an `extra_functionality` constraint.

- The myopic option can now be used together with different clustering for the generators and the network. The existing renewable capacities are split evenly among the regions in every country [#144].

- Add optional function to use `geopy` to locate entries of the Hotmaps database of industrial sites with missing location based on city and country, which reduces missing entries by half. It can be activated by setting `industry: hotmaps_locate_missing: true`, takes a few minutes longer, and should only be used if spatial resolution is coarser than city level.

Performance and Structure

- Extended use of `multiprocessing` for much better performance (from up to 20 minutes to less than one minute).

- Handle most input files (or base directories) via `snakemake.input`.

- Use of `mock_snakemake` from PyPSA-Eur.

- Update `solve_network` rule to match implementation in PyPSA-Eur by using `n.ilopf()` and remove outdated code using `pyomo`. Allows the new setting to skip iterated impedance updates with `solving: options: skip_iterations: true`.

- The component attributes that are to be overridden are now stored in the folder `data/override_component_attrs` analogous to `pypsa/component_attrs`. This reduces verbosity and also allows circumventing the `n.madd()` hack for individual components with non-default attributes. This data is also tracked in the Snakefile. A function `helper.override_component_attrs` was added that loads this data and can pass the overridden component attributes into `pypsa.Network()`.

- Add various parameters to `config.default.yaml` which were previously hardcoded inside the scripts (e.g. energy reference years, BEV settings, solar thermal collector models, geomap colours).

- Removed stale industry demand rules `build_industrial_energy_demand_per_country` and `build_industrial_demand`. These are superseded with more regionally resolved rules.

- Use simpler and shorter `gdf.sjoin()` function to allocate industrial sites from the Hotmaps database to onshore regions. This change also fixes a bug: The previous version allocated sites to the closest bus, but at country borders (where Voronoi cells are distorted by the borders), this had resulted in e.g. a Spanish site close to the French border being wrongly allocated to the French bus if the bus center was closer.

- Retrofitting rule is now only triggered if endogeneously optimised.

- Show progress in build rules with `tqdm` progress bars.

- Reduced verbosity of `Snakefile` through directory prefixes.

- Improve legibility of `config.default.yaml` and remove unused options.

- Use the country-specific time zone mappings from `pytz` rather than a manual mapping.

- A function `add_carrier_buses()` was added to the `prepare_network` rule to reduce code duplication.

- In the `prepare_network` rule the cost and potential adjustment was moved into an own function `maybe_adjust_costs_and_potentials()`.

- Use `matplotlibrc` to set the default plotting style and backend.

- Added benchmark files for each rule.

- Consistent use of `__main__` block and further unspecific code cleaning.

- Updated data bundle and moved data bundle to zenodo.org ([10.5281/zenodo.5546517](#)).

Bugfixes and Compatibility

- Compatibility with `atlite>=0.2`. Older versions of `atlite` will no longer work.

- Corrected calculation of "gas for industry" carbon capture efficiency.

- Implemented changes to `n.snapshot_weightings` in PyPSA v0.18.0.

- Compatibility with `xarray` version 0.19.

- New dependencies: `tqdm`, `atlite>=0.2.4`, `pytz` and `geopy` (optional). These are included in the environment specifications of PyPSA-Eur v0.4.0.

Many thanks to all who contributed to this release!

2.8.4 PyPSA-Eur-Sec 0.5.0 (21st May 2021)

This release includes improvements to the cost database for building retrofits, carbon budget management and wildcard settings, as well as an important bugfix for the emissions from land transport.

This release is known to work with PyPSA-Eur Version 0.3.0 and Technology Data Version 0.2.0.

Please note that the data bundle has also been updated.

New features and bugfixes:

- The cost database for retrofitting of the thermal envelope of buildings has been updated. Now, for calculating the space heat savings of a building, losses by thermal bridges and ventilation are included as well as heat gains (internal and by solar radiation). See the section retro for more details on the retrofitting module.

- For the myopic investment option, a carbon budget and a type of decay (exponential or beta) can be selected in the `config.yaml` file to distribute the budget across the `planning_horizons`. For example, `cb40ex0` in the `{sector_opts}` wildcard will distribute a carbon budget of 40 GtCO2 following an exponential decay with initial growth rate 0.

- Added an option to alter the capital cost or maximum capacity of carriers by a factor via `carrier+factor` in the `{sector_opts}` wildcard. This can be useful for exploring uncertain cost parameters. Example: `solar+c0.5` reduces the `capital_cost` of solar to 50% of original values. Similarly `solar+p3` multiplies the `p_nom_max` by 3.

- Rename the bus for European liquid hydrocarbons from `Fischer-Tropsch` to `EU oil`, since it can be supplied not just with the Fischer-Tropsch process, but also with fossil oil.

- Bugfix: The new separation of land transport by carrier in Version 0.4.0 failed to account for the carbon dioxide emissions from internal combustion engines in land transport. This is now treated as a negative load on the atmospheric carbon dioxide bus, just like aviation emissions.

- Bugfix: Fix reading in of `pypsa-eur/resources/powerplants.csv` to PyPSA-Eur Version 0.3.0 (use column attribute name `DateIn` instead of old `YearDecommissioned`).

- Bugfix: Make sure that `Store` components (battery and H2) are also removed from PyPSA-Eur, so they can be added later by PyPSA-Eur-Sec.

Thanks to Lisa Zeyen (KIT) for the retrofitting improvements and Marta Victoria (Aarhus University) for the carbon budget and wildcard management.

2.8.5 PyPSA-Eur-Sec 0.4.0 (11th December 2020)

This release includes a more accurate nodal disaggregation of industry demand within each country, fixes to CHP and CCS representations, as well as changes to some configuration settings.

It has been released to coincide with PyPSA-Eur Version 0.3.0 and Technology Data Version 0.2.0, and is known to work with these releases.

New features:

- The Hotmaps Industrial Database is used to disaggregate the industrial demand spatially to the nodes inside each country (previously it was distributed by population density).

- Electricity demand from industry is now separated from the regular electricity demand and distributed according to the industry demand. Only the remaining regular electricity demand for households and services is distributed according to GDP and population.

- A cost database for the retrofitting of the thermal envelope of residential and services buildings has been integrated, as well as endogenous optimisation of the level of retrofitting. This is described in the paper Mitigating heat demand peaks in buildings in a highly renewable European energy system. Retrofitting can be activated both exogenously and endogenously from the `config.yaml`.

- The biomass and gas combined heat and power (CHP) parameters `c_v` and `c_b` were read in assuming they were extraction plants rather than back pressure plants. The data is now corrected in Technology Data Version 0.2.0 to the correct DEA back pressure assumptions and they are now implemented as single links with a fixed ratio of electricity to heat output (even as extraction plants, they were always sitting on the backpressure line in simulations, so there was no point in modelling the full heat-electricity feasibility polygon). The old assumptions underestimated the heat output.

- The Danish Energy Agency released new assumptions for carbon capture in October 2020, which have now been incorporated in PyPSA-Eur-Sec, including direct air capture (DAC) and post-combustion capture on CHPs, cement kilns and other industrial facilities. The electricity and heat demand for DAC is modelled for each node (with heat coming from district heating), but currently the electricity and heat demand for industrial capture is not modelled very cleanly (for process heat, 10% of the energy is assumed to go to carbon capture) - a new issue will be opened on this.

- Land transport is separated by energy carrier (fossil, hydrogen fuel cell electric vehicle, and electric vehicle), but still needs to be separated into heavy and light vehicles (the data is there, just not the code yet).

- For assumptions that change with the investment year, there is a new time-dependent format in the `config.yaml` using a dictionary with keys for each year. Implemented examples include the CO2 budget, exogenous retrofitting share and land transport energy carrier; more parameters will be dynamised like this in future.

- Some assumptions have been moved out of the code and into the `config.yaml`, including the carbon sequestration potential and cost, the heat pump sink temperature, reductions in demand for high value chemicals, and some BEV DSM parameters and transport efficiencies.

- Documentation on *Supply and demand* options has been added.

Many thanks to Fraunhofer ISI for opening the hotmaps database and to Lisa Zeyen (KIT) for implementing the building retrofitting.

2.8.6 PyPSA-Eur-Sec 0.3.0 (27th September 2020)

This releases focuses on improvements to industry demand and the generation of intermediate files for demand for basic materials. There are still inconsistencies with CCS and waste management that need to be improved.

It is known to work with PyPSA-Eur v0.1.0 (commit bb3477cd69), PyPSA v0.17.1 and technology-data v0.1.0. Please note that the data bundle has also been updated.

New features:

- In previous version of PyPSA-Eur-Sec the energy demand for industry was calculated directly for each location. Now, instead, the production of each material (steel, cement, aluminium) at each location is calculated as an intermediate data file, before the energy demand is calculated from it. This allows us in future to have competing industrial processes for supplying the same material demand.

- The script `build_industrial_production_per_country_tomorrow.py` determines the future industrial production of materials based on today's levels as well as assumed recycling and demand change measures.

- The energy demand for each industry sector and each location in 2015 is also calculated, so that it can be later incorporated in the pathway optimization.

- Ammonia production data is taken from the USGS and deducted from JRC-IDEES's "basic chemicals" so that it ammonia can be handled separately from the others (olefins, aromatics and chlorine).

- Solid biomass is no longer allowed to be used for process heat in cement and basic chemicals, since the wastes and residues cannot be guaranteed to reach the high temperatures required. Instead, solid biomass is used in the paper and pulp as well as food, beverages and tobacco industries, where required temperatures are lower (see DOI:10.1002/er.3436 and DOI:10.1007/s12053-017-9571-y).

- National installable potentials for salt caverns are now applied.

- When electricity distribution grids are activated, new industry electricity demand, resistive heaters and micro-CHPs are now connected to the lower voltage levels.

- Gas distribution grid costs are included for gas boilers and micro-CHPs.

- Installable potentials for rooftop PV are included with an assumption of 1 kWp per person.

- Some intermediate files produced by scripts have been moved from the folder `data` to the folder `resources`. Now `data` only includes input data, while `resources` only includes intermediate files necessary for building the network models. Please note that the data bundle has also been updated.

- Biomass potentials for different years and scenarios from the JRC are generated in an intermediate file, so that a selection can be made more explicitly by specifying the biomass types from the `config.yaml`.

2.8.7 PyPSA-Eur-Sec 0.2.0 (21st August 2020)

This release introduces pathway optimization over many years (e.g. 2020, 2030, 2040, 2050) with myopic foresight, as well as outsourcing the technology assumptions to the technology-data repository.

It is known to work with PyPSA-Eur v0.1.0 (commit bb3477cd69), PyPSA v0.17.1 and technology-data v0.1.0.

New features:

- Option for pathway optimization with myopic foresight, based on the paper Early decarbonisation of the European Energy system pays off (2020). Investments are optimized sequentially for multiple years (e.g. 2020, 2030, 2040, 2050) taking account of existing assets built in previous years and their lifetimes. The script uses data on the existing assets for electricity and building heating technologies, but there are no assumptions yet for existing transport and industry (if you include these, the model will greenfield them). There are also some outstanding issues on e.g. the distribution of existing wind, solar and heating technologies within each country. To use myopic foresight, set `foresight : 'myopic'` in the `config.yaml` instead of the default `foresight : 'overnight'`. An example configuration can be found in `config.myopic.yaml`. More details on the implementation can be found in *Myopic transition path*.

- Technology assumptions (costs, efficiencies, etc.) are no longer stored in the repository. Instead, you have to install the technology-data database in a parallel directory. These assumptions are largely based on the Danish Energy Agency Technology Data. More details on the installation can be found in *Installation*.

- Logs and benchmarks are now stored with the other model outputs in `results/run-name/`.

- All buses now have a `location` attribute, e.g. bus `DE0 3 urban central heat` has a `location` of `DE0 3`.

- All assets have a `lifetime` attribute (integer in years). For the myopic foresight, a `build_year` attribute is also stored.

- Costs for solar and onshore and offshore wind are recalculated by PyPSA-Eur-Sec based on the investment year, including the AC or DC connection costs for offshore wind.

Many thanks to Marta Victoria for implementing the myopic foresight, and Marta Victoria, Kun Zhu and Lisa Zeyen for developing the technology assumptions database.

2.8.8 PyPSA-Eur-Sec 0.1.0 (8th July 2020)

This is the first proper release of PyPSA-Eur-Sec, a model of the European energy system at the transmission network level that covers the full ENTSO-E area.

It is known to work with PyPSA-Eur v0.1.0 (commit bb3477cd69) and PyPSA v0.17.0.

We are making this release since in version 0.2.0 we will introduce changes to allow myopic investment planning that will require minor changes for users of the overnight investment planning.

PyPSA-Eur-Sec builds on the electricity generation and transmission model PyPSA-Eur to add demand and supply for the following sectors: transport, space and water heating, biomass, industry and industrial feedstocks. This completes the energy system and includes all greenhouse gas emitters except waste management, agriculture, forestry and land use.

PyPSA-Eur-Sec was initially based on the model PyPSA-Eur-Sec-30 (Version 0.0.1 below) described in the paper Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system (2018) but it differs by being based on the higher resolution electricity transmission model PyPSA-Eur rather than a one-node-per-country model, and by including biomass, industry, industrial feedstocks, aviation, shipping, better carbon management, carbon capture and usage/sequestration, and gas networks.

PyPSA-Eur-Sec includes PyPSA-Eur as a snakemake subworkflow. PyPSA-Eur-Sec uses PyPSA-Eur to build the clustered transmission model along with wind, solar PV and hydroelectricity potentials and time series. Then PyPSA-Eur-Sec adds other conventional generators, storage units and the additional sectors.

2.8.9 PyPSA-Eur-Sec 0.0.2 (4th September 2020)

This version, also called PyPSA-Eur-Sec-30-Path, built on PyPSA-Eur-Sec 0.0.1 (also called PyPSA-Eur-Sec-30) to include myopic pathway optimisation for the paper Early decarbonisation of the European energy system pays off (2020). The myopic pathway optimisation was then merged into the main PyPSA-Eur-Sec codebase in Version 0.2.0 above.

This model has its own github repository and is archived on Zenodo.

2.8.10 PyPSA-Eur-Sec 0.0.1 (12th January 2018)

This is the first published version of PyPSA-Eur-Sec, also called PyPSA-Eur-Sec-30. It was first used in the research paper Synergies of sector coupling and transmission reinforcement in a cost-optimised, highly renewable European energy system (2018). The model covers 30 European countries with one node per country. It includes demand and supply for electricity, space and water heating in buildings, and land transport.

It is archived on Zenodo.

2.8.11 Release Process

- Finalise release notes at `doc/release_notes.rst`.
- Update version number in `doc/conf.py` and `*config.*.yaml`.
- Make a `git commit`.
- Tag a release by running `git tag v0.x.x`, `git push`, `git push --tags`. Include release notes in the tag message.
- Make a GitHub release, which automatically triggers archiving by zenodo.
- Send announcement on the PyPSA mailing list.

To make a new release of the data bundle, make an archive of the files in `data` which are not already included in the git repository:

```
data % tar pczf pypsa-eur-sec-data-bundle.tar.gz eea/UNFCCC_v23.csv switzerland-sfoe␣
↪biomass eurostat-energy_balances-* jrc-idees-2015 emobility WindWaveWEC_GLTB.xlsx␣
↪myb1-2017-nitro.xls Industrial_Database.csv retro/tabula-calculator-calcsetbuilding.
↪csv nuts/NUTS_RG_10M_2013_4326_LEVL_2.geojson h2_salt_caverns_GWh_per_sqkm.geojson
```

2.9 Limitations

While the benefit of an openly available, functional and partially validated model of the European energy system is high, many approximations have been made due to missing data. The limitations of the dataset are listed below, both as a warning to the user and as an encouragement to assist in improving the approximations.

This list of limitations is incomplete and will be added to over time.

See also the GitHub repository issues.

- **Electricity transmission network topology:** The grid data is based on a map of the ENTSO-E area that is known to contain small distortions to improve readability. Since the exact impedances of the lines are unknown, approximations based on line lengths and standard line parameters were made that ignore specific conducting choices for particular lines. There is no openly available data on busbar configurations, switch locations, transformers or reactive power compensation assets.

- **Assignment of electricity demand to transmission nodes:** Using Voronoi cells to aggregate load and generator data to transmission network substations ignores the topology of the underlying distribution network, meaning that assets may be connected to the wrong substation.

- **Incomplete information on existing assets:** Approximations have been made for missing data, including: existing distribution grid capacities and costs, existing space and water heating supply, existing industry facilities, existing transport vehicle fleets.

- **Exogenous pathways for transformation of transport and industry:** To avoid penny-switching the transformation of transport and industry away from fossil fuels is determined exogenously.

- **Industry materials production constant and inelastic:** For industry, the production of different materials per country is assumed to remain constant and no industry demand elasticity is included in the modelled.

- **Energy demand distribution within countries:** Assumptions have been made about the distribution of demand in each country proportional to population and GDP that may not reflect local circumstances. Openly available data on load time series may not correspond to the true vertical load and is not spatially disaggregated; assuming, as we have done, that the load time series shape is the same at each node within each country ignores local differences.

- **Hydro-electric power plants:** The database of hydro-electric power plants does not include plant-specific energy storage information, so that blanket values based on country storage totals have been used. Inflow time series are based on country-wide approximations, ignoring local topography and basin drainage; in principle a full hydrological model should be used.

- **International interactions:** Border connections and power flows to Russia, Belarus, Ukraine, Turkey and Morocco have not been taken into account; islands which are not connected to the main European system, such as Malta, Crete and Cyprus, are also excluded from the model.

- **Demand sufficiency:** Further measures of demand reduction may be possible beyond the assumptions made here.

Licence

The code in PyPSA-Eur-Sec is released as free software under the MIT license, see LICENSE. However, different licenses and terms of use may apply to the various input data.