Closing the Loop: Integrating Material Needs of Energy Technologies into Energy System Models

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Abstract— **The transition to a climate-neutral energy system demands large-scale renewable generation expansion, which requires substantial amounts of bulk materials like steel, cement, and polymers. The production of these materials represents an additional energy demand for the system, creating an energy-material feedback loop. Current energy system models lack a complete representation of this feedback loop. Material requirements of energy system transformation have been studied in a retrospective approach, not allowing them as a consideration in system design.**

To address this gap, we integrate bulk material demand and production as endogenous factors into energy system optimization using PyPSA-Eur. Our approach links infrastructure expansion with industrial energy needs to achieve a minimum-cost equilibrium.

Applying this model to Germany's transition to climate neutrality by 2045, we find that accounting for material needs increases annual bulk material demands by 3–9 %, shifts preferences from solar to wind and from local production of hydrogen to ship imports, and shows distinct industrial process route choices. These findings suggests that energy-material feedbacks should be considered in energy system design when moving to more domestic production of energy technologies.

Index Terms–Energy-material nexus, energy system modelling, industry defossilization.

I. INTRODUCTION

Meeting climate neutrality targets in the energy sector requires expanding large capacities of renewable technologies. This drives substantial demand for both critical raw materials and bulk materials such as steel, cement, and polymers [1]. For energy-intensive bulk materials, this creates a bidirectional energy-material feedback loop: energy is needed to produce materials, and materials are needed to build energy technologies [2]. Unless met entirely through imports, these material demands can influence optimal system design, particularly in resource- and emissions-constrained scenarios where small changes in demand may cause significant cost increases.

Currently, many technologies essential for a net-zero European energy system, such as solar panels and fuel cells, are largely imported [3]. However, the EU's Net-Zero Industry Act aims to localize value chains to reduce dependency and enhance resilience [3]. These goals underscore the importance of analyzing energy system design with full energy-material feedbacks.

Most research focuses on critical materials ([4], [5], review by [2]) which are relevant due to their supply risks and limited availability [6]. This is modelled by supply constraints or multi-criteria optimization (e.g. [5]). In contrast, the challenge with bulk materials is that they are required in large volumes—e.g., wind turbines are composed of 70–72 % concrete and 24–25 % steel [1], and their production is highly energy- and emissions-intensive [7], creating additional challenges for climate-neutral transitions. Considering the effect of bulk material demands in energy system models thus requires modelling energy demand and emissions related to their production.

Material needs of the energy transition have been quantified with retrospective approaches, multiplying technology expansion from fixed energy scenarios with material intensity factors to estimate demand (e.g., [4]; review by [2]). This approach does not allow consideration of material needs in the energy system design. Some integrate industrial production to reflect industry energy use but treat material demands as exogenous (e.g., [8], [9], [10]). Only a few studies capture full feedbacks by endogenizing material demand and supply, but they focus on a single material such as lithium [11] or copper [12], or include bulk materials but with limited energy system resolution [13].

We propose a novel approach to integrate bulk material demand and production into energy system optimization, explicitly modeling feedbacks in both directions (see fig. 1). Our approach extends existing reasearch by introducing material demand as an additional criterion in technology selection (e.g., wind turbines, direct air capture or heat pumps), and by co-optimizing industry process selection to provide these materials domestically. The main objective is to find out whether domestic material production for the energy system transformation leads to a different optimal system design than imported technology and materials.

To achieve this, we enhance the open-source energy system model PyPSA-Eur [14] with two modifications. First, we directly link material demands to energy infrastructure expansion. Second, we model industrial processes for bulk materials, making pro-

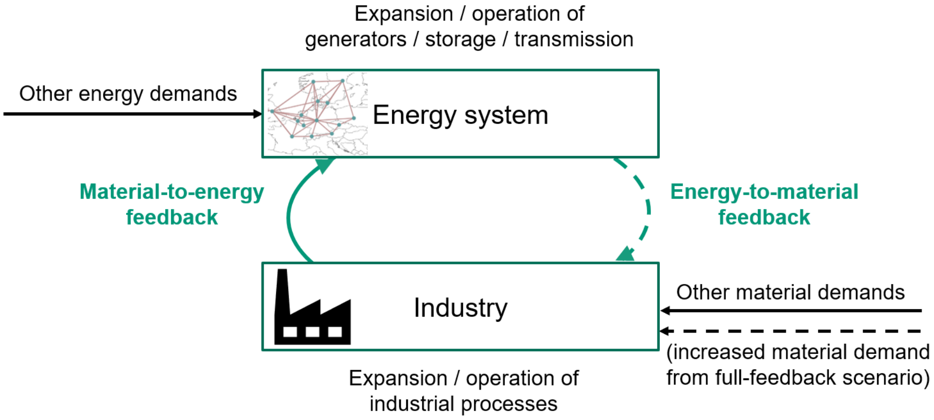

Fig. 1. Feedbacks between industry and energy system in the optimization. Material-to-energy feedback: energy carrier demand from operation of industry processes (all scenarios). Energy-to-material feedback: material demand from energy technology expansion (only domestic production scenarios). Other demands include demands from other sectors, e.g. buildings and transport. The increased material demand is only included in the increased-material reference (*100 %, not linked*) and set to the material demand of the scenario with full feedback (*100 % domestic*). For separate representation of cross-sectoral links in scenarios see appendix fig. 7.

duction routes and fuel choices endogenous.

We apply this feedback-loop model for Germany's energy and industrial transformation to climate neutrality by 2045. In a reference scenario, material demands linked to energy system expansion are not considered, corresponding to the assumption that 0 % of materials are produced domestically in Germany. The other scenarios stepwise increase the domestic production share to 25, 50, 75 and 100 % respectively. In an additional reference scenario, the material demands are increased to the level of the *100 % domestic* scenario, but without linking material demands to technology expansion (*100 %, not linked*). The feedbacks included in the different scenarios are shown in fig. 1.

The following section (II) describes the optimization problems of the compared scenarios. Section III compares the optimization results of the different scenarios regarding material demands and technology choices in industry and energy system. Main findings, limitations and future work for our study are discussed in the section IV.

II. METHODOLOGY

We develop an optimization model of the energy-intensive industry, comprising options for producing the bulk materials steel, cement, and high-value chemicals HVC, as well as for providing industrial process heat at three temperature levels. This model is coupled to the energy system model PyPSA-Eur [14] for Germany and countries with a direct power transfer link. A more detailed description of the industry and energy system models as well as a full mathematical model formulation is given the appendix in section IV.

The objective function minimizes annual system costs for expansion and operation of technologies, under emission and resource caps, in an overnight (no pathway), greenfield (no current technology capacities considered) approach for the year 2045. System costs consist of total costs of the industry sector and the energy system. The decision variables are the expansion and operation of industry processes, generators, transmission, and conversion technologies, and storage, summed for all nodes of the network and time steps of the one-year horizon. Costs consist of annualized investment costs, operational costs, and costs for consuming resources. The operational costs of the industry processes include raw material costs and exclude energy carrier costs, but industrial energy carrier demands induce costs in the energy system to provide the energy carriers. Equally, in the domestic production scenarios, the capital costs of technology expansion do not include costs for steel, cement and HVC, but demand for these materials induce costs in the industry sector to produce them (and costs in energy system for providing related industrial energy demands). This avoids double-counting of material costs addressed in [2]. In the scenarios with partial domestic production (*25, 50, 75 % domestic*), capital costs only exclude the share of domestically produced materials. In the reference scenarios, no material demands of energy system technologies are domestically produced, thus capital costs include bulk material costs.

In all scenarios, industry and energy system operation are connected through the energy balance as schematically shown in fig. 1. It defines for each energy carrier, that generation, storage, conversion, and transmission within the energy system must meet the exogenous demand plus the endogenous consumption by industry and conversion processes. The exogenous demand consists of demand from the non-industry sectors (e.g., buildings, transport) and aggregated demands of further, not explicitly modelled industry subsectors (e.g., pulp and paper, food processing, etc., based on 2021 data from the JRC-IDEES database [7] and from [15]). Electricity and hydrogen can be exchanged between the countries when networks are expanded in the optimization, and hydrogen ship imports are enabled at a price of 84 €/MWh.

The material balances ensure that demand for each material (steel, cement and HVC) is met by industrial production. In the reference scenarios, an exogenous material demand is set. In the other scenarios annualized material demands per capacity build-up of energy system technologies must additionally be served. Material demands are annualized by distributing them equally over the lifetimes of the technologies. This corresponds to the assumption of constant rebuilding of technologies after 2045. The per-capacity material demands of the technologies are shown in the appendix.

Limits for resource consumption and emissions are set jointly for industry and energy system, thus they compete for certain resources, such as biomass, waste, and CO_2 storage capacity, and waste. The emission limit is set to zero, corresponding to the limit of the German climate law for 2045.

III. RESULTS AND DISCUSSION

A. Material demands and production

Fig. 2 shows the resulting total demand for cement, HVC and steel in the different scenarios and their resulting respective process routes. Material demand increases endogenously as energy system technologies expand according to domestic production shares. The increased-material scenario (*100 %, not linked*) sets material demands exogenously, matching the *100 % domestic* scenario, but without linking demand to technology expansion. Compared to the reference (*0 % domestic*), 100 % domestic production increases material demands by 3 % (cement), 3 % (HVC), and 9 % (steel). Steel demand is most affected due to its high share in energy system technology materials (see material factors in appendix).

Production routes remain unchanged for cement (low-clinker mixtures with carbon capture) and steel (recycling up to limits set by steel scrap availability, and H_2 direct reduction). HVC production relies on chemical and mechanical recycling up to the secondary material limit. Methanol-to-olefins dominates in the 0–50 % local production scenarios, while steam cracking with synthetic naphtha (from Fischer-Tropsch) partially replaces it in the 75–100 % scenarios. The *increased-material* reference scenario (100 %, not linked) continues to rely entirely on methanol-to-olefins for primary production, like in the *0 - 50 % domestic* scenarios.

Resulting process heat technology choices are the same for low- and high-temperature heat in all scenarios, but differ in the medium-temperature range. For low-temperature heat, industrial heat pumps are used in all scenarios. For medium temperature heat, around half comes from furnaces fueled with bioenergy plus carbon capture and storage (BECCS) and half from H_2-fueled furnaces in the reference scenario. In the *100 % domestic* scenario, the ratio shifts towards biomass furnaces with BECCS (78 %). In the *100 %, not linked* reference, this ratio shift towards biomass furnaces is less pronounced (60 %). High-temperature heat is entirely provided by biomass furnaces with BECCS in all scenarios, with total heat demand increasing as domestic material production rises.

B. Energy system

The energy system must meet additional demands induced by increased local material production. This results in a cost-minimal equilibrium, as technology expansion further induces material demand. Fig. 3 shows expansion for electricity generation across scenarios. Instead of additional generator expansion, most of the additional energy demand is met through H_2 imports by ship (fig. 4). Renewable capacities remain stable for most technologies or even decreases for utility solar, which has a high material demand relative to capacity factors (see material factors in appendix).

For dispatchable generators, H_2 turbine and fuel cell capacities increase, while gas and biomass combined heat and power plant capacities (CHPs) decline with increasing shares of domestic production. This also reduces heat supplied to district heating networks from CHPs. Instead, heat is increasingly sourced from waste heat from Fischer-Tropsch and fuel cells in the *75 %* and *100 % domestic* scenarios, along with expanded gas boilers, heat pumps, and direct electric heaters.

Compared to the *increased-material* reference scenario, the *100 % domestic* scenario results in lower overall generator capacity expansion and greater reliance on H_2 ship imports (36 TWh compared to 27 TWh). H_2 ship imports come from outside the modelled system and do not induce a material demand in the modelled system; instead, the material costs are reflected in the import price. This leads to reduced deployment of material-intensive solar and slightly lower onshore wind capacity. Additionally, less CHP capacity is built, with increased deployment of H_2 turbines and fuel cells.

C. Energy-to-material feedback

The annualized per-technology material demand in the *100 % domestic* scenario is compared to the material demands of the system design in the *100 %, not linked* scenario in fig. 5. In the latter scenario, material demands for technologies are not a consideration in energy system design. Thus, this comparison allows to assess the preference shift in technology choice when their materials demands are linked, comparing additional endogenous material demands linked to technology expansion versus additional exogenous material demand at the same level but not linked to technology expansion.

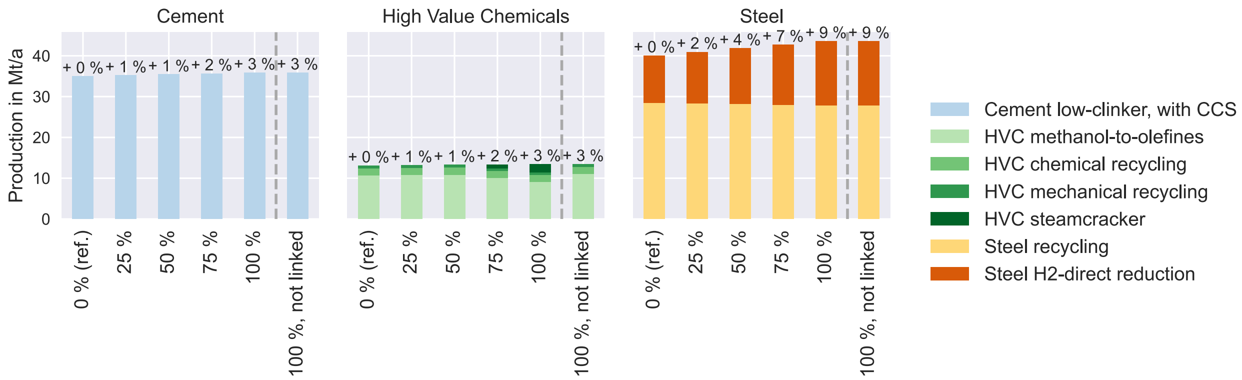

Fig. 2. Material demand and production by process route at the German node in 2045, by scenario. The scenarios vary in the percentage of domestically produced materials (here: domestically = in Germany). The numbers on the bars describe the increase in material demand compared to the reference scenario. The dashed line separates the increased-material reference (*100 %, not linked*) which differs in the optimization problem: material demands are set exogenously, matching the levels of the *100 % domestic* scenario, but are not induced by the expansion of technologies.

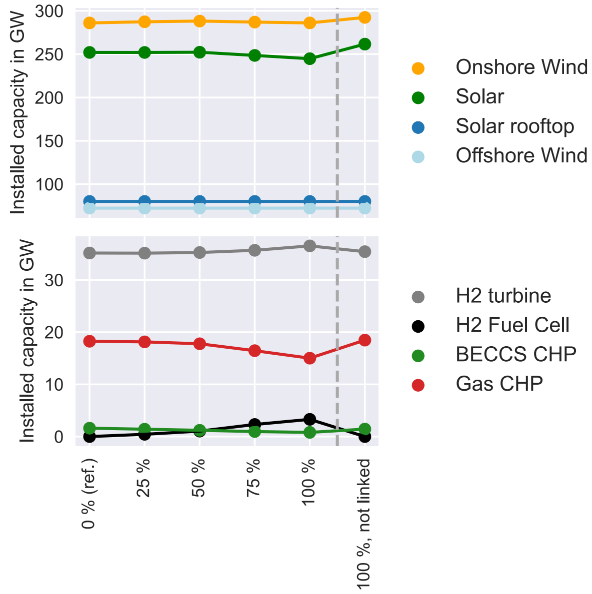

Fig. 3. Installed capacities by scenario for renewable generators (top) and dispatchable generators (bottom). Note: different y-axis scales.

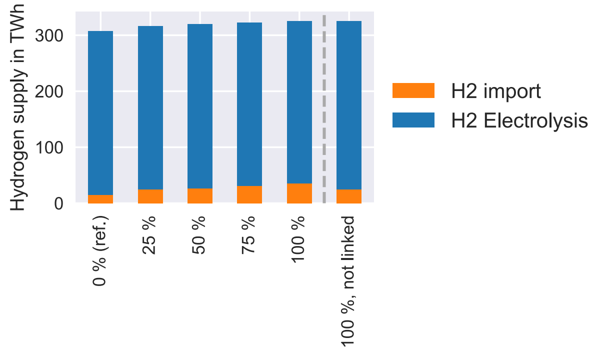

Fig. 4. Hydrogen supply by scenario.

The *100 % domestic* scenario builds a more material-efficient system. For all three materials, total demand is higher in the exogenous material scenario, particularly for steel (additional 94 kt / year). This is primarily driven by increased deployment of utility solar. Additionally, more onshore wind expansion, BECCS and gas CHPs are built. These technologies drive higher material demands than the heat pumps, H_2 turbines and fuel cells preferred in the *100 % domestic* scenario.

The amount of materials contained in technologies at the German node in the *100 % domestic* scenario is shown in fig. 6, in comparison to the amount of material demand calculated for today's installed solar and wind generators in Germany. The 2045 amounts, compared to 2015, increase by factor 6 (steel), 5 (cement) and 9 (HVC), mostly used in onshore wind, solar and offshore wind generators.

IV. CONCLUSION

We present a method to integrate energy-material feedbacks into energy system models. To achieve this, we extended the sector-coupled PyPSA-Eur model by incorporating (1) an industry module representing production routes for steel, cement, and HVC, along with process heat technologies, and (2) material factors that endogenously link technology expansion to material demand. This approach addresses a gap identified in previous research [2].

We apply this method to a model of Germany and countries with a direct power link. Our results reveal two key effects of incorporating a full energy-material feedback loop in optimization. First, technology expansion drives bulk material demands by 3–9 %, which drives higher energy demand. Second, compared to a scenario with exogenously increased material demands, endogenous material feedback shifts technology preferences from solar to onshore wind and from electrolysis to H_2 imports. Further tech-

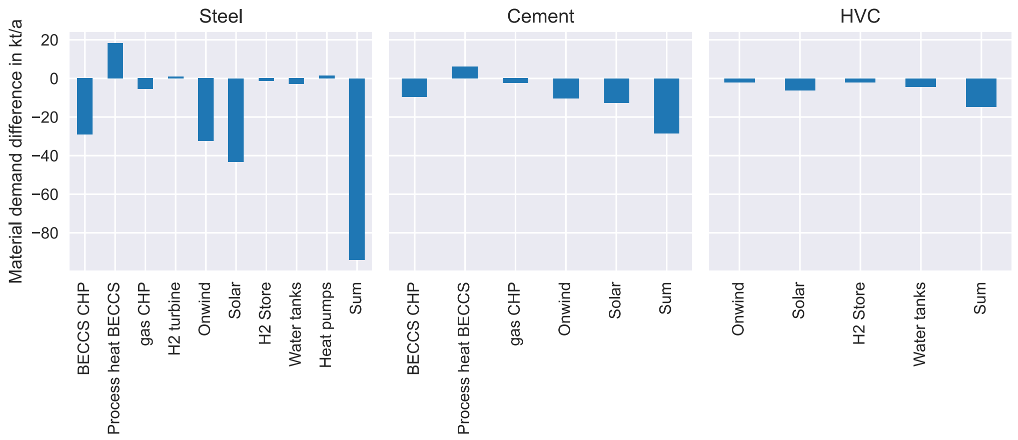

Fig. 5. System material demand by technology of the *100 % domestic* scenario minus (hypothetical) system material demand of the *100 %, not linked* reference. Negative values mean higher material demand in the latter scenario. The sum includes all technologies, while for the single technologies, only the most relevant technologies inducing material differences higher than 500 kt/y are shown.

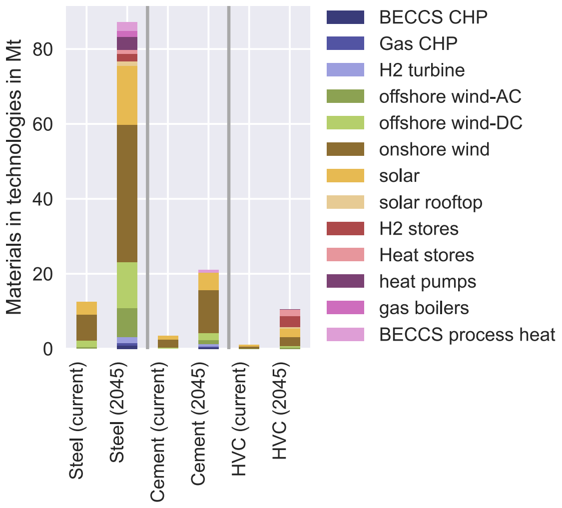

Fig. 6. Material contained in resulting technology capacities in the *100 % domestic* scenario for 2045, compared to current material contained in solar and wind technologies, both for Germany

nology choice differences occur in HVC production, process heat generation, and dispatchable electricity supply, leading to a system design with reduced material needs. Our findings emphasize the importance of accounting for energy-material interactions in cost-optimal system design.

The method presented in this paper has several limitations. First, material demands for technology construction are distributed evenly over a plant's lifetime, an assumption that holds only if technologies are replaced at a constant rate. Second, the adjustment of technology capacity costs to exclude bulk material expenses is based on their current market prices, but the actual proportion of capital costs attributed to bulk materials may be different and change over time. Lastly, due to data limitations, material factors for some technologies were unavailable and were approximated using values from comparable technologies, and we did not include sub-technologies (e.g. wind turbines with or without permanent magnet as in [5]), assuming that the effect on structural materials is limited.

Our study can be extended in several ways. First, we apply a greenfield and overnight (no pathway, no current technologies) optimization for a climate-neutral system. While this represents energy-material feedbacks in the optimal system design, it cannot represent material requirements before 2045 to build up the climate-neutral system. Future work could apply our method in a pathway study. Second, our analysis focuses on bulk materials as structural components of energy technologies. While steel, cement, and HVC are the most energy-intensive materials in Germany, further research could expand to other materials such as copper and aluminum, and additional technologies like grids and electric vehicles. Third, our study focuses on Germany as a proof-of-concept. While effects are already visible at this national scope, extending the model to European level could offer valuable insights, allowing to consider different local conditions for renewable generation and exchange of energy and bulk materials between countries.

V. ACKNOWLEDGMENTS

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APPENDIX I
SCENARIOS

Fig. 7 shows the modelled links in different scenarios in comparison. Endogenous and exogenous aspects in the scenarios are summarized in table I.

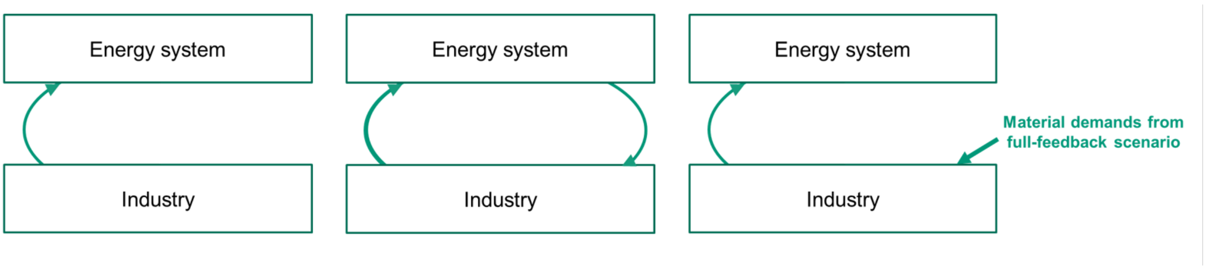

Fig. 7. Links included in the optimization of the scenarios: Reference (left), *100 % domestic* (middle) and *increased-material*s reference (right)

TABLE I
ENDOGENOUS AND EXOGENOUS (INPUT) PARTS OF MODELS IN THE COMPARED SCENARIOS.

Scenarios	**Endogenous**	**Exogenous (Inputs)**
all	Energy system and industry technology expansion and operation	Material demands not linked to technology expansion, Energy demands not linked to industry
reference (0 % domestic production)		additional: zero material demands for technology expansion
Domestic production (25 / 50 / 75 / 100 %)	Additional: material demands linked to technology expansion, according to domestic share	
Increased-material reference		Additional: material demands taken from 100% domestic scenario

APPENDIX II
MATERIAL FACTORS

Material factors for steel, cement and HVC are taken from [16] (electricity generators), [17] (process and space heat technologies), [18] (solar rooftop, storage technologies) and [19] (direct air capture). Material factors are shown in fig. 8 and fig. 9. Comparing the material factors for renewable generators, offshore wind generators show the highest bulk material demands per capacity, followed by onshore wind and solar. However, the actual maximum power output for these generators per capacity differ. When comparing the material demands per maximum average energy output of the technologies (i.e. running the technologies for one year at their maximum capacity factors), offshore wind AC remains the most material-intensive generator, followed by solar, offshore wind DC and onshore wind. For dispatchable generators, those equipped with carbon capture show substancially higher material factors.

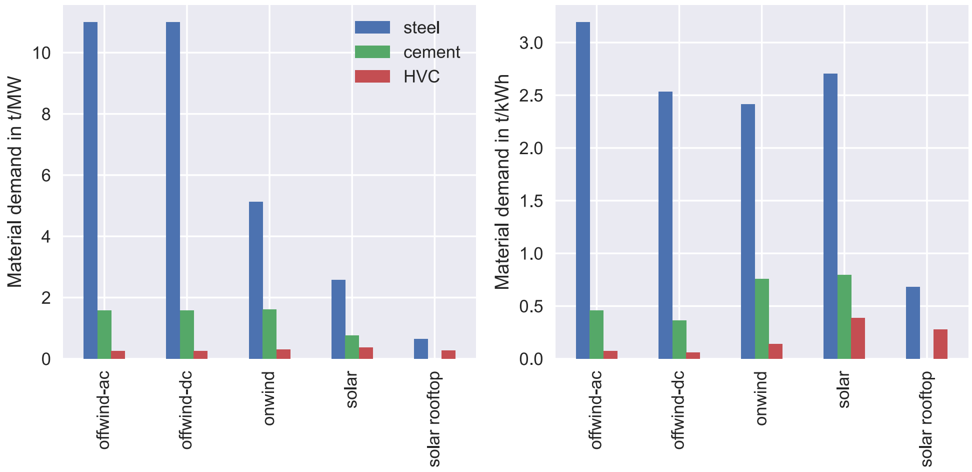

Fig. 8. Annualized material demand with equal distributed material demand over technology lifetime, relative to capacity (left) and maximum energy output (right). Maximum energy output means that the technologies are assumed to run at maximum capacity factor all year (no curtailment).

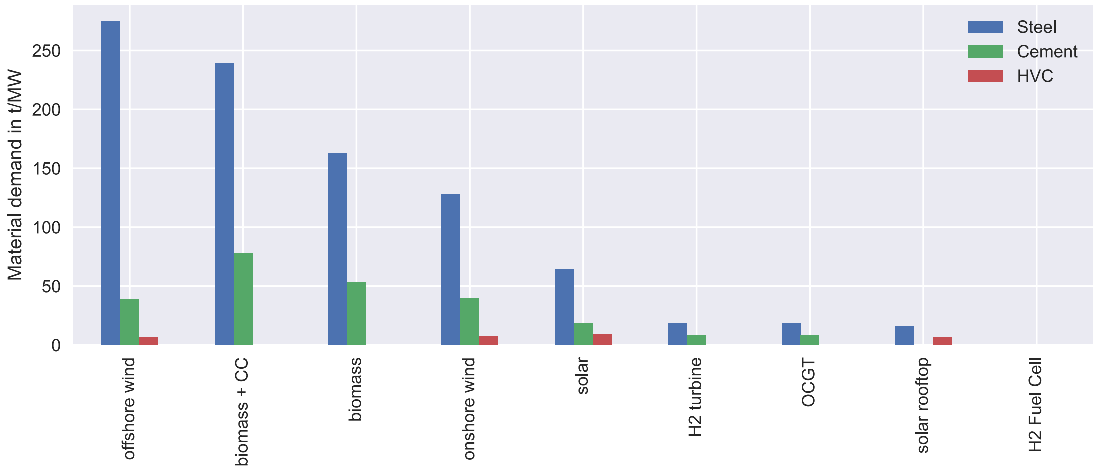

Fig. 9. Annualized material demand with equal distributed material demand over technology lifetime, for electricity generators, relative to capacity.

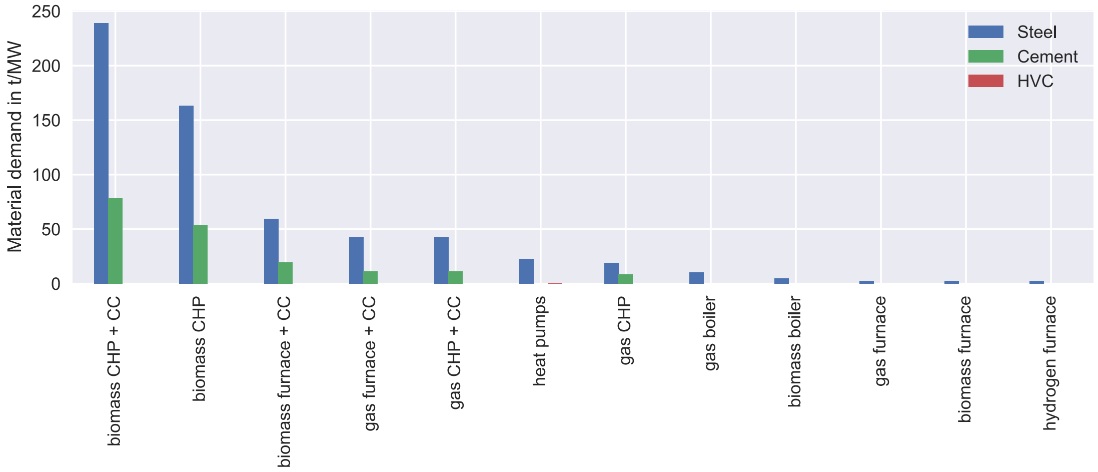

Fig. 10. Annualized material demand with equal distributed material demand over technology lifetime, for heat generators, relative to heat generation capacity.

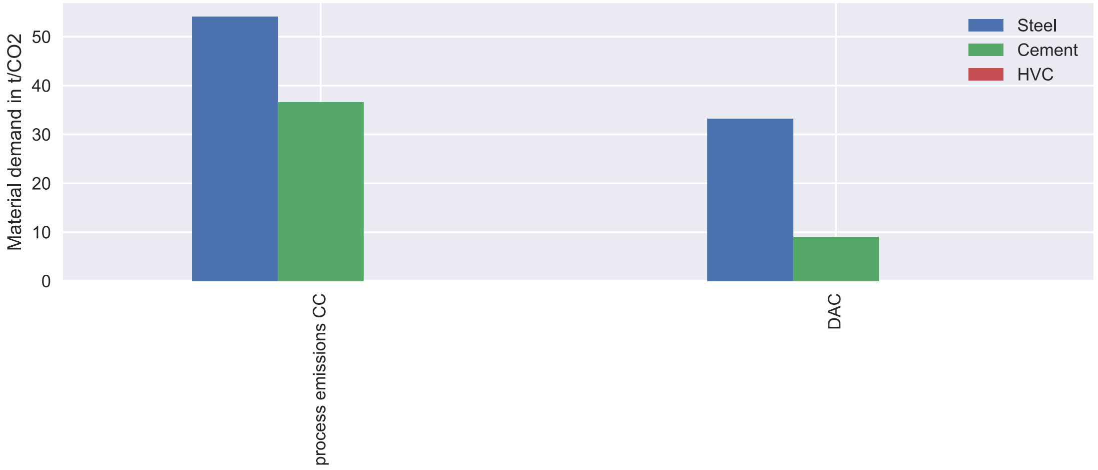

Fig. 11. Annualized material demand with equal distributed material demand over technology lifetime, for carbon capture technologies, relative to CO_2 capture capacity.

APPENDIX III
RESULTS: H_2 USE

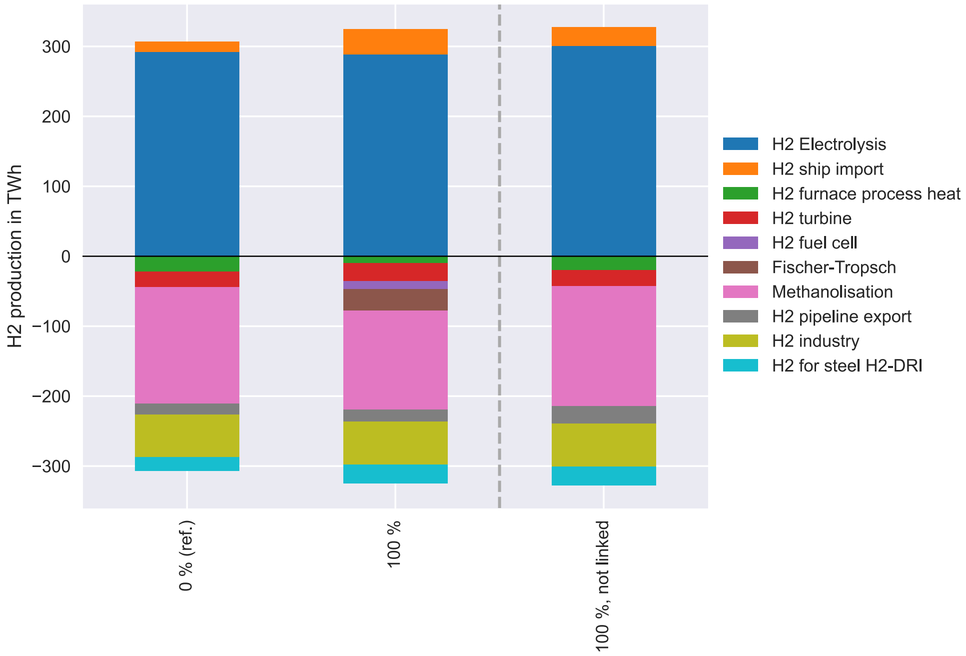

Fig. 12. Hydrogen production (positive values) and use (negative values) in the reference (0 %), *100 % domestic* (100 %), and increased-material reference (100 %, not linked) scenarios.

fig.12 shows H_2 use and production at the German node for the reference scenario, the *100 % domestic* production scenario and the reference scenario with material demands from the *100 % domestic* production scenario. H_2 use increases compared to the reference scenario (307 TWh) in the two 100 % scenarios to similar levels (325 TWh *100 % domestic* and 327 TWh *increased-material reference*). Compared to the reference scenario, the *100 % domestic* scenario increases H_2 use for steel production (since more steel is produced) and additional Fischer-Tropsch (for HVC production) and additional H_2 turbines and fuel cells, while consumption by methanolisation and furnaces decrease (more biomass furnaces instead). In the increased-material reference scenario (100 %, not linked), compared to the reference scenario, technology choice remains equal with just more capacity expansion due to increased material demand, i.e. more H_2 for steel production (27 TWh compared to 20 TWh) and methanolisation (171 TWh compared to 166 TWh), but slightly less for H_2 furnaces (20 TWh compared to 22 TWh) due to a shift to biomass furnaces with BECCS. Also, more pipeline exports of H_2 to neighboring countries (16 TWh reference, 17 TWh *100 % domestic*, 25 TWh *increased-material reference*). Compared to the 100 % linked scenario, differences are that the production route for HVC remains methanol-to-olefines completely, such that only methanolisation and H_2 for steel use increases, and that no additional dispatchable electricity technology is expanded (fuel cell) and the H_2 for process heat is kept.

The increased H_2 demand compared to the reference is met by increased ship imports in the *100 % domestic* production scenario and with increased electrolysis in the *100 % domestic* production scenario. In the local production scenario, electricity demand of electrolysis requires more expansion of generators requiring materials requiring industry expansion requiring generators expansion. In the unlinked scenario, the generators expansion does not have further effects. Ship imports of H_2 do not have an effect on capacity expansion or material demands since they come from outside the system.

APPENDIX IV

DETAILED MODEL DESCRIPTION

Industry model: The industry model characterizes each process route and each process heat technology option with specific emissions, demand for energy carriers, process heat and raw materials (e.g., steel scrap or plastic waste for the recycling routes), and operating and annualised investment costs. The demand for process heat is partly endogenous because it depends on the expanded and operated process routes for bulk material production. Model inputs are bulk material demands (steel, cement, HVC) and process heat demand at different temperature levels for all industry branches.

Energy system model: The energy system model represents Germany and countries with a direct power transfer link, which is the same scope as used in the PyPSA-Ariadne version focusing on Germany [20], at a resolution of one node per country. Technologies for the conversion, transmission, and storage of multiple energy carriers (electricity, H_2, methane, naphtha and oil, methanol) and heat are expanded and operated. H_2 can be generated by electrolysis and exchanged between the countries via pipelines, or imported via ship. The exogenous industrial energy demand at the German node is replaced by attaching the industry model. The non-industrial energy demand, e.g., for buildings and transport, and the demand for industrial sectors other than steel, cement and HVC are exogenous inputs.

The operational costs of the industry processes do not include energy carrier costs, but energy carrier demands induce costs in the energy system to provide the energy carriers.

The capital costs of technologies include the costs for imported materials, while costs for locally produced materials are excluded, since they are indirectly represented by the necessary build-up and operation of industry processes (and energy system technologies). For the full-feedback case, the capital costs of technologies in PyPSA-Eur are corrected by subtracting material costs. The material costs are calculated based on material factors of a technology and commodity prices. These prices are taken from [21] and [22] and [23].

In the reference scenario, technology expansion at the German node and in neighboring countries is endogenous. In all other scenarios, technology capacities in neighboring countries are fixed to prevent shifts from material-demand-linked technologies in Germany to non-material-demand-linked technologies abroad. We do so to make the impact of the energy-to-material feedback identifiable.

objective function:

$$\min_{g,f,i,\overline{g},\overline{l},\overline{f},\overline{i},\overline{b^{ch}},\overline{b^{d}},\overline{e}} \quad z^{esm} + z^{ind} \tag{1}$$

with:

$$z^{ind} = \sum_{p\in\mathcal{P}} \sum_{n\in\mathcal{N}} \sum_{t\in\mathcal{T}} i_{p,n,t} \left(C_p^{\text{op,ind}} + \sum_{r\in\mathcal{R}} R_{p,r}^{\text{ind}} C_r^{\text{res}} \right) \quad + \sum_{n\in\mathcal{N}} \sum_{p\in\mathcal{P}} \overline{i}_{p,n} C_p^{\text{inv,ind}} \tag{2}$$

$$\begin{aligned} z^{esm} =& \sum_{k\in\mathcal{K}} \sum_{n\in\mathcal{N}} \left(\sum_{t\in\mathcal{T}} g_{k,n,t} C_k^{\text{op,gen}} + \overline{g}_{k,e,n} C_k^{\text{inv,gen}} \right) \\ &+ \sum_{s\in\mathcal{S}} \sum_{n\in\mathcal{N}} \left(\overline{b}_{s,n}^{ch} C_s^{\text{inv,stor,ch}} + \overline{b}_{s,n}^{d} C_s^{\text{inv,stor,d}} + \overline{e}_{s,n} C_s^{\text{inv,stor,en}} \right) \\ &+ \sum_{e\in\mathcal{E}} \sum_{n,m\in\mathcal{N}} \overline{l}_{e,n,m} C_{e,n,m}^{\text{inv,tr}} \\ &+ \sum_{c\in\mathcal{C}} \sum_{n\in\mathcal{N}} \left(\sum_{t\in\mathcal{T}} f_{c,n,t} \left(C_c^{\text{op,conv}} + \sum_{r\in\mathcal{R}} R_{c,r}^{\text{conv}} C_r^{\text{res}} \right) + \overline{f}_{c,n} C_c^{\text{inv,conv}} \right) \end{aligned} \tag{3}$$

TABLE II

VARIABLES

Variable	**Index Sets**	**Description**	**Unit**
$\overline{g}$	$\mathcal{K}, \mathcal{N}$	Installed capacity of generators	MW
$\overline{l}$	$\mathcal{E}, \mathcal{N}, \mathcal{N}$	Transmission line capacity node to node	MW
$\overline{i}$	$\mathcal{P}, \mathcal{N}$	Installed capacity of industrial processes	t/y
$\overline{f}$	$\mathcal{C}, \mathcal{N}$	Installed capacity of conversion technologies	MW
$\overline{b}^{ch}$	$\mathcal{S}, \mathcal{N}$	Installed charging capacity of storage	MW
$\overline{b}^{d}$	$\mathcal{S}, \mathcal{N}$	Installed discharging capacity of storage	MW
$\overline{e}$	$\mathcal{S}, \mathcal{N}$	Installed energy capacity of storage	MWh
b^{ch}	$\mathcal{S}, \mathcal{N}, \mathcal{T}$	charging of storage	MW
b^{d}	$\mathcal{S}, \mathcal{N}, \mathcal{T}$	discharging of storage	MW
e	$\mathcal{S}, \mathcal{N}$	energy of storage	MWh
g	$\mathcal{K}, \mathcal{E}, \mathcal{N}, \mathcal{T}$	Power production by generators	MWh
f	$\mathcal{C}, \mathcal{N}, \mathcal{T}$	Conversion flow	MWh
i	$\mathcal{P}, \mathcal{N}, \mathcal{T}$	Industry processes operation	t
l	$\mathcal{E}, \mathcal{N}, \mathcal{N}, \mathcal{T}$	Transmission of energy carrier from first node to second node	MWh
z^{ind}	-	Annual costs of industry	€
z^{esm}	-	Annual costs of energy system	€

Energy balance:

$$D_{\mathrm{e,n,t}} = \sum_{p\in\mathcal{P}} i_{\mathrm{p,n,t}} \cdot E_{\mathrm{p,e}} + \sum_{c\in\mathcal{C}} f_{\mathrm{c,n,t}} \cdot E_{\mathrm{c,e}} + \sum_{k\in\mathcal{K}} g_{\mathrm{k,n,t}} \cdot E_{\mathrm{k,e}} + \sum_{m\in\mathcal{N}} (l_{\mathrm{e,m,n,t}} - l_{\mathrm{e,n,m,t}}) + \sum_{s\in\mathcal{S}} (b^{\mathrm{d}}_{\mathrm{s,n,t}} - b^{\mathrm{ch}}_{\mathrm{s,n,t}}) \cdot E_{\mathrm{s,e}} \quad \forall e \in \mathcal{E}, \forall n \in \mathcal{N}, \forall t \in \mathcal{T} \tag{4}$$

Material balance:

$$D^{\mathrm{mat}}_{\mathrm{m,n}} = \sum_{p\in\mathcal{P}} \sum_{t\in\mathcal{T}} i_{\mathrm{p,n,t}} \cdot M^{\mathrm{ind}}_{\mathrm{p,m}} + \sum_{k\in\mathcal{K}} \overline{g}_{k,n} \cdot M_{\mathrm{k,m}} + \sum_{s\in\mathcal{S}} \overline{e}_{s,n} \cdot M_{\mathrm{s,m}} + \sum_{c\in\mathcal{C}} \overline{f}_{c,n} \cdot M_{\mathrm{c,m}} \qquad \forall n \in \mathcal{N}, \forall m \in \mathcal{M} \tag{5}$$

Resource constraint:

$$\sum_{p\in\mathcal{P}} \sum_{t\in\mathcal{T}} i_{p,n,t} \cdot R_{p,r} + \sum_{c\in\mathcal{C}} \sum_{t\in\mathcal{T}} f_{c,n,t} \cdot R_{c,r} \leq R^{max}_{r} \quad \forall r \in \mathcal{R}, \forall n \in \mathcal{N} \tag{6}$$

Emission constraint:

$$\sum_{p\in\mathcal{P}} \sum_{t\in\mathcal{T}} i_{p,n,t} \cdot X_p + \sum_{c\in\mathcal{C}} \sum_{t\in\mathcal{T}} f_{c,n,t} \cdot X_c + \sum_{k\in\mathcal{K}} \sum_{t\in\mathcal{T}} g_{k,n,t} \cdot X_k \leq 0 \quad \forall n \in \mathcal{N} \tag{7}$$

Operation constraints: The operation of all technologies is constrained by their capacities. The generation of renewable powerplants is further constrained by their time- and location-dependent capacity factors CF, which are defined between 0 and 1 as a fraction of capacity.

$$f_{c,n,t} \leq \overline{f}_{c,n} \qquad \forall\, c \in \mathcal{C},\ \forall\, n \in \mathcal{N}, \forall\, t \in \mathcal{T} \tag{8}$$

$$g_{k,n,t} \leq \overline{g}_{k,n} \cdot CF_{k,n,t} \qquad \forall\, k \in \mathcal{K},\ \forall\, n \in \mathcal{N}, \forall\, t \in \mathcal{T} \tag{9}$$

$$l_{e,m,n,t} \leq \overline{l}_{e,m,n} \qquad \forall\, e \in \mathcal{E}, \forall\, m \in \mathcal{N},\ \forall\, n \in \mathcal{N}, \forall\, t \in \mathcal{T} \tag{10}$$

Capacity limits:

$$0 \leq \overline{f}_{c,n} \leq \overline{F}^{max}_{c,n} \qquad \forall\, c \in \mathcal{C},\ \forall\, n \in \mathcal{N} \tag{11}$$

$$\overline{G}^{start}_{k,n} \leq \overline{g}_{k,n} \leq \overline{G}^{max}_{k,n} \qquad \forall\, k \in \mathcal{K},\ \forall\, n \in \mathcal{N} \tag{12}$$

$$0 \leq \overline{l}_{e,m,n} \leq \overline{L}^{max}_{e,m,n} \qquad \forall\, e \in \mathcal{E},\ \forall\, n \in \mathcal{N}, \forall\, m \in \mathcal{M} \tag{13}$$

Transmission between nodes only possible for transmittable carriers:

$$\overline{L}^{max}_{e,m,n} = 0 \forall e \in \mathcal{E} \notin \mathcal{E}^{tr}, \forall m, n \in \mathcal{N} \tag{14}$$

We apply the optimal linear power flow method described in the PyPSA documentation [14]. Further constraints are described in the PyPSA documentation (*Storage Unit constraints, Generator constraints, Passive branch flows*). If not said otherwise, the default parameters of PyPSA-Eur are kept, e.g., investment costs, capacity factors, energy carrier limits.

TABLE III

SETS AND THEIR ELEMENTS. HIGHT = HIGH-TEMPERATURE, MEDIUMT = MEDIUM-TEMPERATURE, LOWT = LOW-TEMPERATURE.

Set	**Description**	**Elements**
$\mathcal{P}$	Industrial processes	'steel EAF', 'steel H_2-DRI+EAF', 'steel ISW', 'steel NG-DRI+EAF', 'hvc steamcracker', 'hvc chemical recycling', 'hvc mechanical recycling', 'hvc electric steamcracker', 'hvc MtO', 'cement CEM I', 'cement CEM II/C-M', 'cement CEM II/AB-M', 'cement CEM II C/ Q-L', 'lowT industry solid biomass', 'lowT industry solid biomass CC', 'lowT industry methane', 'lowT industry methane CC', 'lowT industry heat pump', 'lowT industry electricity', 'solid biomass for mediumT industry', 'solid biomass for mediumT industry CC', 'gas for mediumT industry', 'gas for mediumT industry CC', 'hydrogen for mediumT industry', 'gas for highT industry', 'gas for highT industry CC', 'hydrogen for highT industry', 'process emissions CC', 'gas for industry CC', 'mediumT industry electricity', 'plasma for highT industry', 'solid biomass for highT industry', 'highT industry solid biomass CC', 'coal for highT industry', 'waste for highT industry'
$\mathcal{M}$	Materials	Steel, cement, HVC
$\mathcal{S}$	Storage technologies	'CO_2 store', 'gas store', 'H_2 store', 'battery', 'residential rural water tanks', 'services rural water tanks', 'residential urban decentral water tanks', 'services urban decentral water tanks', 'urban central water tanks', 'methanol', 'oil', 'home battery', 'highT industry heat', 'mediumT industry heat', 'lowT industry heat'
$\mathcal{T}$	Timesteps	0, 3, ..., 2920 (1 year in 3h resolution)
$\mathcal{N}$	Nodes in the system	1 node per country for Germany + countries with direct power links
$\mathcal{C}$	Conversion technologies	'OCGT', 'H_2 Electrolysis', 'H_2 Fuel Cell', 'Sabatier', 'SMR CC', 'SMR', heat pump, resistive heater, gas boiler, gas CHP', gas CHP CC', 'biogas to gas', 'solid biomass CHP', ' solid biomass CHP CC', 'biomass boiler', 'biomass to liquid', 'BioSNG', 'methanolisation', 'Fischer-Tropsch', 'DAC', 'BioSNG CC', 'solid biomass to hydrogen CC', 'biomass to liquid CC', 'electrobiofuels', 'solid biomass to electricity', 'solid biomass to electricity CC', 'waste CHP CC', 'waste CHP', 'H_2 turbine'
$\mathcal{R}$	Resources	'biogas', 'solid biomass', 'municipal solid waste', 'plastic waste', 'packaging waste', 'steel scrap'
$\mathcal{K}$	Generation technologies	onshore wind, offshore wind, solar, solar rooftop, run-of-river, hydropower
$\mathcal{A}$	All technologies	$K \cup C \cup S \cup P$
$\mathcal{E}$	Energy carriers and heat	electricity, methane, hydrogen, space heat (residential / servives; central / decentral), industry process heat ('lowT industry', 'mediumT industry', 'highT industry'), methanol, oil / naphtha, coal
$\mathcal{E}^{\text{tr}}$	Transmittable energy carriers	Electricity, hydrogen

Secondary material availability for HVC and steel in the year y = 2045 is calculated based on the method applied in [9] and [24]. Materials go to enduses, and become secondary material after the lifetime of the respective enduse $end \in Enduses$. The secondary material secondarymat in year y is $\text{secondarymat}_y = \sum_{end \in \text{Enduses}} (p_{(y-\text{lifetime}_{\text{end}})} \cdot \text{share}_{\text{end}} \cdot \text{recovery}_{\text{end}}$, with p being the production of the material in a specific year.

A. Input and model details

- Ship H_2 imports: We include H_2 import via ship transport to LNG terminals at a constant price of 84 €/MWh (taken from [23]). For the countries in scope, overseas pipeline imports are not an option [23].
- Flexibility of technologies: Industrial processes are modeled with a flat profile, i.e. are not flexible. Some conversion processes allow flexible operation, e.g., electrolysis (rampable 0% to 100% of capacity), methanolisation (50 % to 100 %), Fischer-Tropsch (90 % to 100%), process heat technologies (80 % to 100%), heat pumps and electric heaters and boilers (all 0 % to 100 %), dispatchable electricity generators (all 0 % to 100 %). No vehicle-to-grid is included.
- Exogenous material demand (not from energy technologies): We assume the same material production for Germany in 2045 as today (2021). Thus, effects of industry production moving to other countries or changes in material demand are not considered. This is changed in sensitivity analyses. Sources for material production today: steel and cement from the IDEES-2021 database [7]. The database gives only aggregated basic chemicals demand, so we take methanol and HVC production in Germany from [15].
- Spatial scope and resolution: The energy system model comprises one node per country for Germany and countries with a direct power transmission link (12 ”electricity neighbors” are represented, as in the model version of the Ariadne project [20]). Endogenous process route choice is only applied for the German node, while the simplified industry representation is kept for the other nodes. Process heat provision is

TABLE IV

PARAMETERS

Parameter	Index Sets	Description	Unit
$C^{op,ind}$	$\mathcal{P}$	Operating cost of industrial processes	€/t
$C^{inv,ind}$	$\mathcal{P}$	Investment cost of industrial processes	€/(t/y)
C^{res}	$\mathcal{R}$	Price of resources	€/MWh or €/t
R	$\mathcal{A}$, $\mathcal{R}$	Resource demand of technology	t/t or t/MWh
$C^{op,gen}$	$\mathcal{K}$	Operating cost of generators	€/MWh
$C^{inv,gen}$	$\mathcal{K}$	Investment cost of generators	€/MW
$C^{inv,stor,ch}$	$\mathcal{S}$	Investment cost for storage charging capacity	€/MW
$C^{inv,stor,d}$	$\mathcal{S}$	Investment cost for storage discharging capacity	€/MW
$C^{inv,stor,en}$	$\mathcal{S}$	Investment cost for storage energy capacity	€/MWh
$C^{inv,tr}$	$\mathcal{E},\mathcal{N},\mathcal{N}$	Investment cost for transmission	€/MW
$C^{op,conv}$	$\mathcal{C}$	Operating cost of conversion technologies	€/MWh
R^{max}_{r}	$\mathcal{R}$	Overall resource limit	t or MWh
$C^{inv,conv}$	$\mathcal{C}$	Investment cost of conversion technologies	€/MW
E	$\mathcal{A},\mathcal{E}$	Energy carrier production by technology (- when consumed)	MWh/MWh
M^{ind}	$\mathcal{P},\mathcal{M}$	Material production by technology	t/MWh
M	$\mathcal{A},\mathcal{M}$	Material consumption (- sign) by technology capacity	t/MW
D	$\mathcal{E},\mathcal{N},\mathcal{T}$	Exogenous energy carrier demand	MWh
$D^{non-ind}$	$\mathcal{E},\mathcal{N},\mathcal{T}$	Exogenous non-industrial energy carrier demand	MWh
D^{mat}	$\mathcal{M},\mathcal{N},\mathcal{T}$	Exogenous material demand	t
X	$\mathcal{A}$	Emissions from technology operation	t/MWh
X^{gen}	$\mathcal{K}$	Emissions of generators	t/MWh
$\overline{F}^{max}$	$\mathcal{C},\mathcal{N}$	Capacity limit of conversion technology c at n	MW
$\overline{G}^{max}$	$\mathcal{K},\mathcal{N}$	Capacity limit of generator k at n	MW
G^{start}	$\mathcal{K},\mathcal{N}$	Initial capacity of generator k at n	MW
$\overline{L}^{max}$	$\mathcal{E},\mathcal{N},\mathcal{N}$	Capacity limit of transmission from m to n	MW
CF	$\mathcal{K},\mathcal{N},\mathcal{T}$	Generator capacity factor	-

endogenous for all nodes and industry branches (except for the German node in the soft-linked energy system optimisation where process heat provision is determined in the previous industry optimisation).

- Transmission: Transmission of energy carriers between nodes is only possible for electricity and hydrogen, through the expansion of lines, DC links and pipelines. CO_2, methane, oil / naphtha, and methanol used at the German node must also be provided by technologies at the German node, and resources cannot be imported from other nodes.
- Resource limits: Biomass, emissions and CO_2 storage capacity is limited for Germany. For the other nodes, joint limits are set. Biomass data for Germany and other countries in scope is taken from the JRC-ENSPRESO database, scenario ENS-Med, for the year 2040 [25]. Biomass to liquid and BioSNG are enabled as options. No additional (outside Europe) biomass imports are enabled.
- Temporal resolution and horizon: 3H resolution, 1 year.
- Exogenous energy demands (not from bulk material production): Electricity load for standard electricity applications and space heat (today's level). Additional loads for electric vehicles are added. Electricity demand for other power-to-X technologies is endogenous, e.g., heat pumps, electrolysers, methanolisation. Further exogenous energy demands: oil for aviation and agriculture, H_2 fuel cell, process heat, feedstock and electricity demand for other industry branches than steel, cement and HVC.