

Supplementary Information 1

Carbon dioxide removal enables climate planetary boundary compliance in cost-effective energy-industry transition pathways

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Supplementary figures

LUT-ESTM regional detail

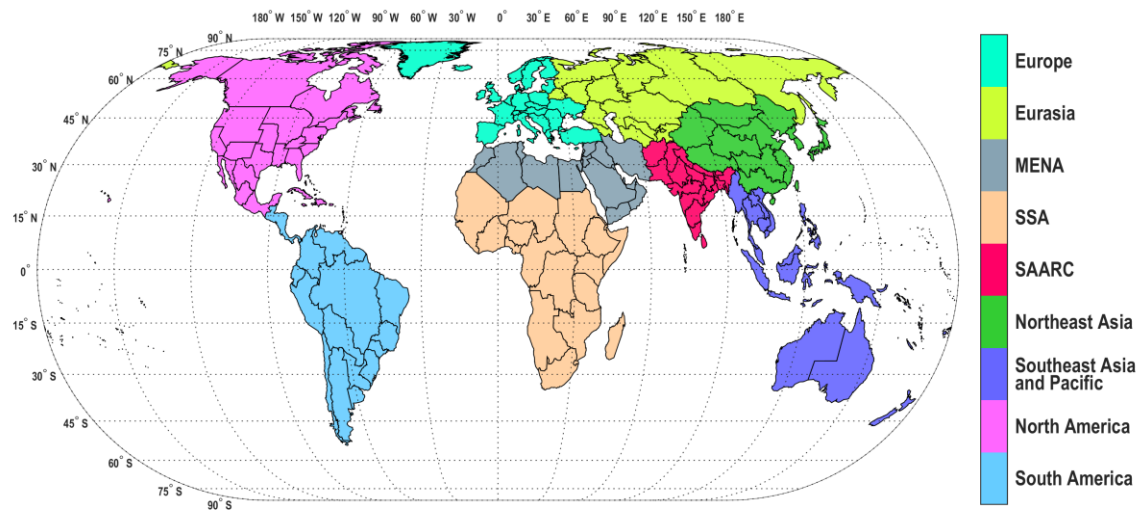


Figure S1. Major regions of LUT-ESTM with a spatial breakdown into 151 regions as an intermediate step between country resolution and major regions used for resource profile modelling.

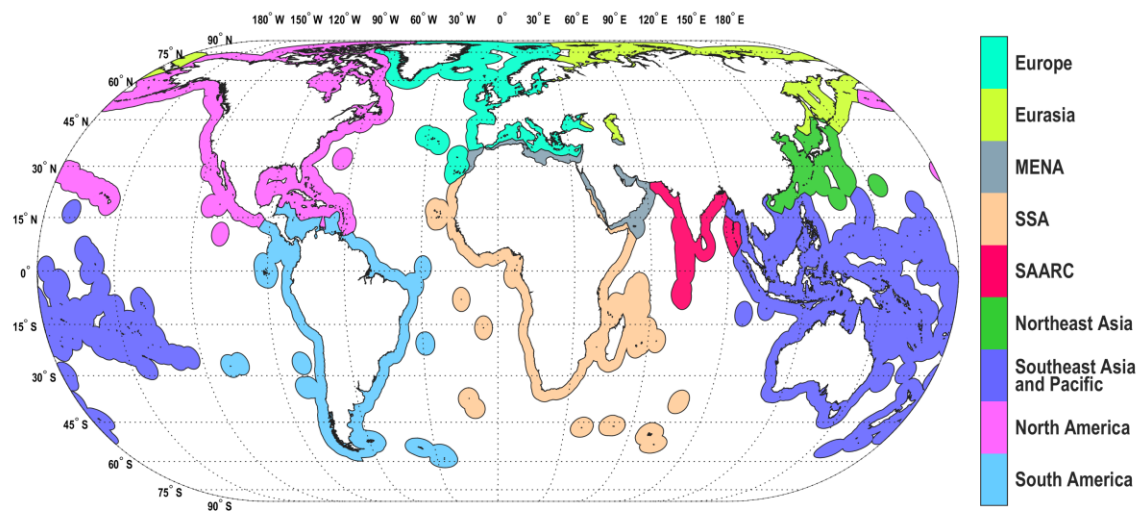


Figure S2. Exclusive economic zones (EEZ) of major regions of LUT-ESTM used for offshore technology potential availability.

CDR portfolios per major region – 1.5°C climate target

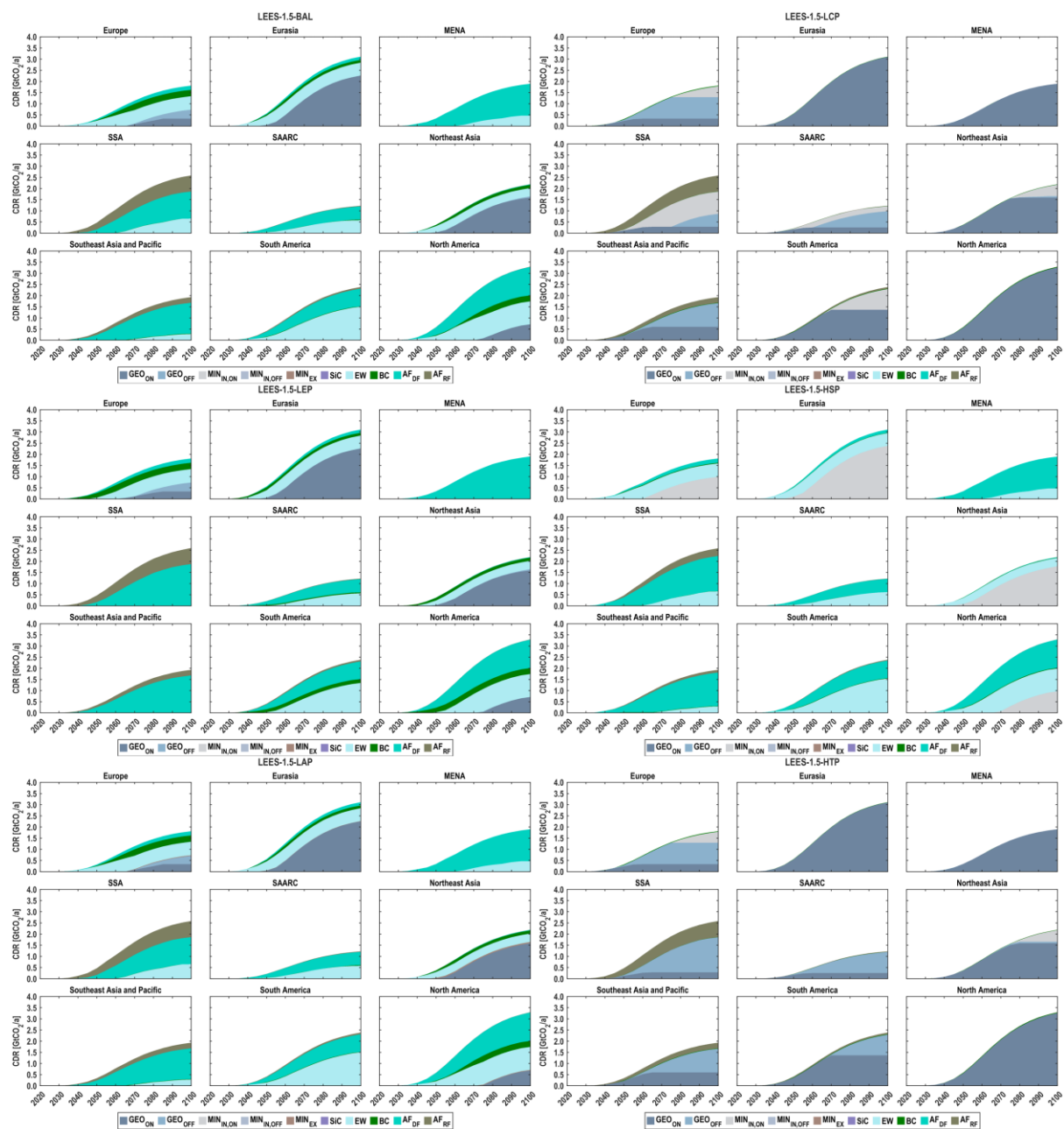


Figure S3. CDR portfolios of 9 major regions for 1.5°C scenarios.

CDR portfolios per major region – 1.0°C climate target

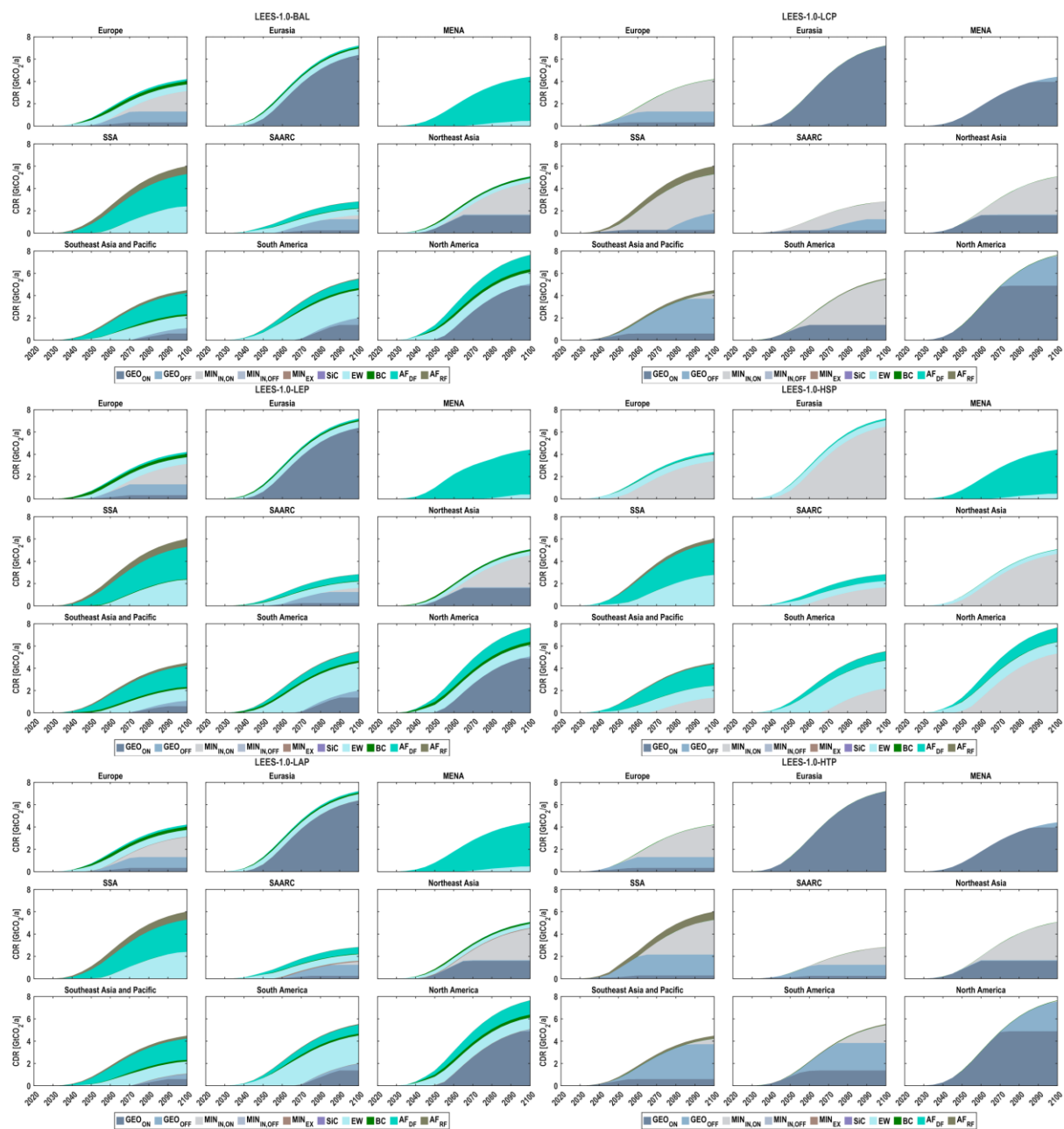


Figure S4. CDR portfolios of 9 major regions for 1.0°C scenarios.

Energy-industry-CDR system transition figures

The full set of transition figures and detailed result files can be found in the extended supplementary material 1 folder in the Zenodo repository with the identifier: [10.5281/zenodo.22041775](https://zenodo.org/records/22041775). The figures are organised by scenario, transition, and map diagrams.

During peer review, the files can be accessed using the following private review link:

https://zenodo.org/records/22041775?token=eyJhbGciOiJIUzUxMiJ9.eyJpZCI6IjVhMjFhNzQyLWI0NjAtNDczOC1iYTcxLWFiNzU5MDE5MzBhNyIsImRhdGEiOiJhYTA2NDIxODI5MTliYjA2ZWQ0ODRmMmQzYzdmNzZkMiJ9.qjluDhGjmJ2jHsl5o_E0-1JzGKvrC5RYRxxg3yp7GopypXAKZbJKDQS643xA5iUOYY9VJyFwXnSMuKpQU0UL-jQ

This link and yellow highlighted text will be removed and the dataset made publicly accessible upon acceptance.

To illustrate the broad set of results and respective visualisation, Figure S5-Figure S23 show exemplary results for the scenario **LEES-1.0-BAL**. The complete figure set covering all evaluated scenarios is available in the public repository as mentioned above.

The figures are separated by global transition figures and regional map diagrams. Map diagrams show regional results for the modelled 9 regions for the years 2030, 2050, and 2100, as presented in the main study. Table S1 gives an overview for provided figures for orientation.

Table S1. Overview on additional figures provided in this supplementary material for orientation.

Figure	Parameter
Figure S5	Levelised cost of electricity (LCOE), levelised cost of final energy and feedstock/non-energy use (LCOFE), total annualised system cost
Figure S6	Electricity generation capacity and electricity generation
Figure S7	Energy storage capacity and energy throughput
Figure S8	Heat generation capacity and heat generation
Figure S9	CO ₂ management; CDR by source, by technology, and demand for CO ₂
Figure S10	Final energy demand and primary energy demand
Figure S11	Levelised cost of electricity (LCOE)
Figure S12	Electricity generation capacity
Figure S13	Electricity storage capacity
Figure S14	Electricity storage throughput
Figure S15	Heat and gas storage capacity and throughput
Figure S16	Hydrogen production capacity and hydrogen production
Figure S17	Heat generation capacity and heat generation
Figure S18	Supply of fuels and chemicals and hydrogen use
Figure S19	Structure of CO ₂ supply for CCS, CCU, and CDR
Figure S20	CDR by technology and CO ₂ source
Figure S21	CCU by CO ₂ source and product

Supplementary figures

Figure S22	Unbalanced and balanced CO ₂ management by sector and fuel for a representative 1.5°C target scenario
Figure S23	Unbalanced and balanced CO ₂ management by sector and fuel for a representative 1.0°C target scenario

Global transition figures

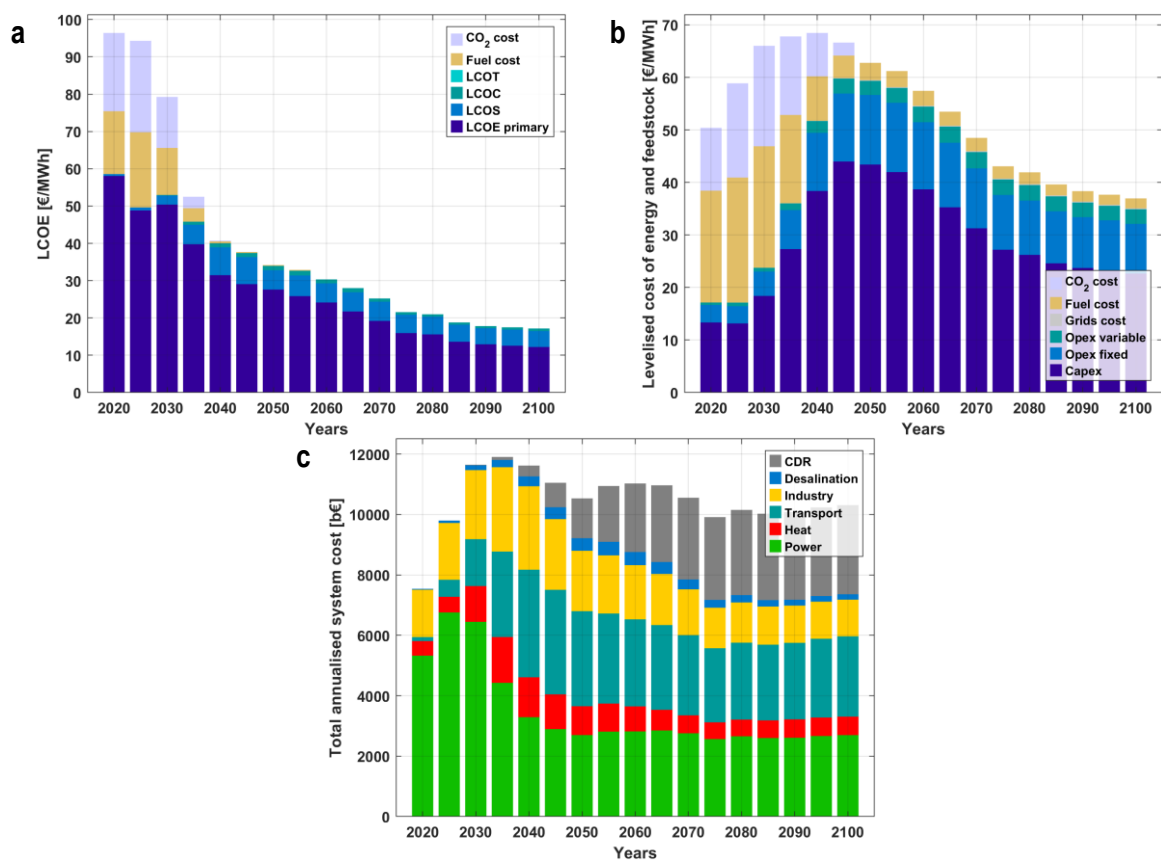


Figure S5. **(a)** Global transition for levelised cost of electricity (LCOE). **(b)** Global transition of levelised cost of energy and feedstock/non-energy use (LCOFE). **(c)** Development of total annualised system cost by sector. Abbreviations: LCOS – levelised cost of storage, LCOC – levelised cost of curtailment, LCOT – levelised cost of transmission, capex – capital expenditures, opex – operational expenditures.

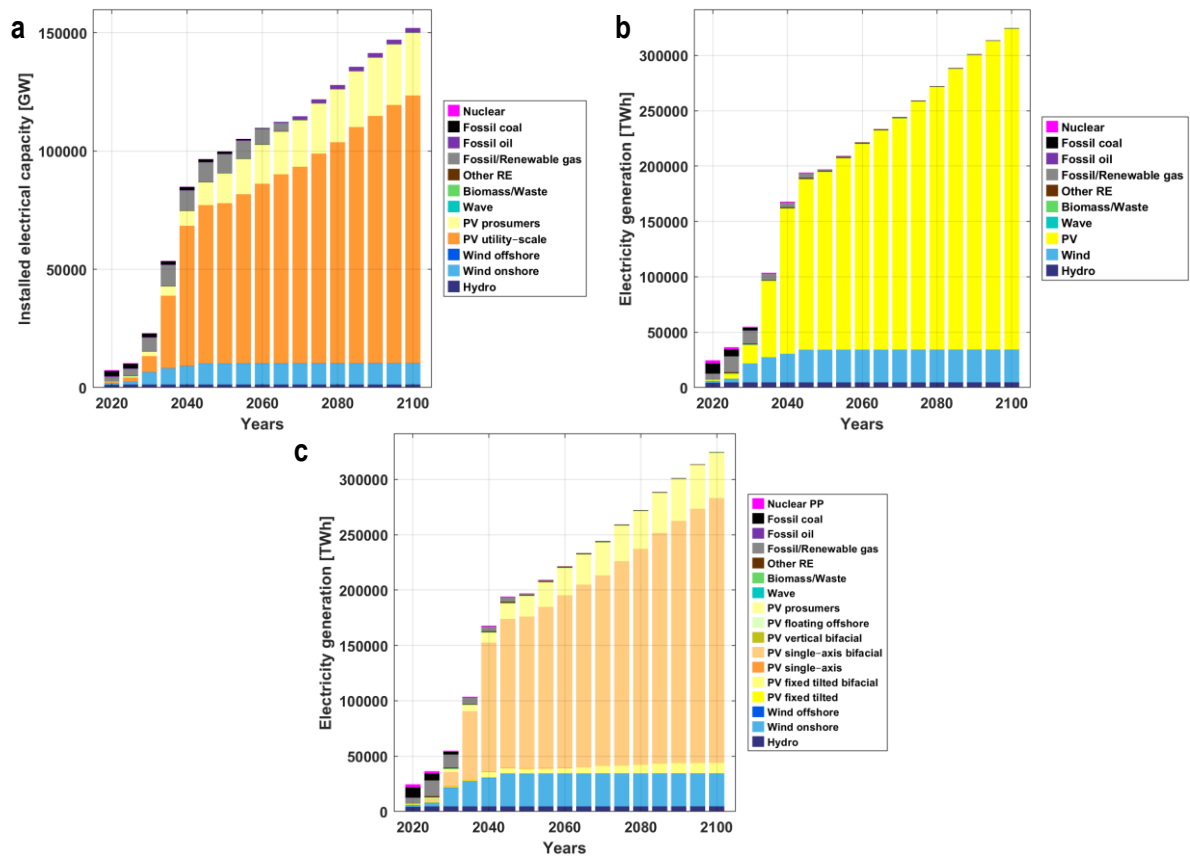


Figure S6. **(a-b)** Global transition for installed capacity for detailed **(a)** and aggregated **(b)** electricity generation capacity. **(c)** Global electricity generation by technology. Abbreviations: RE – renewable energy, PV – photovoltaics, PP – power plant.

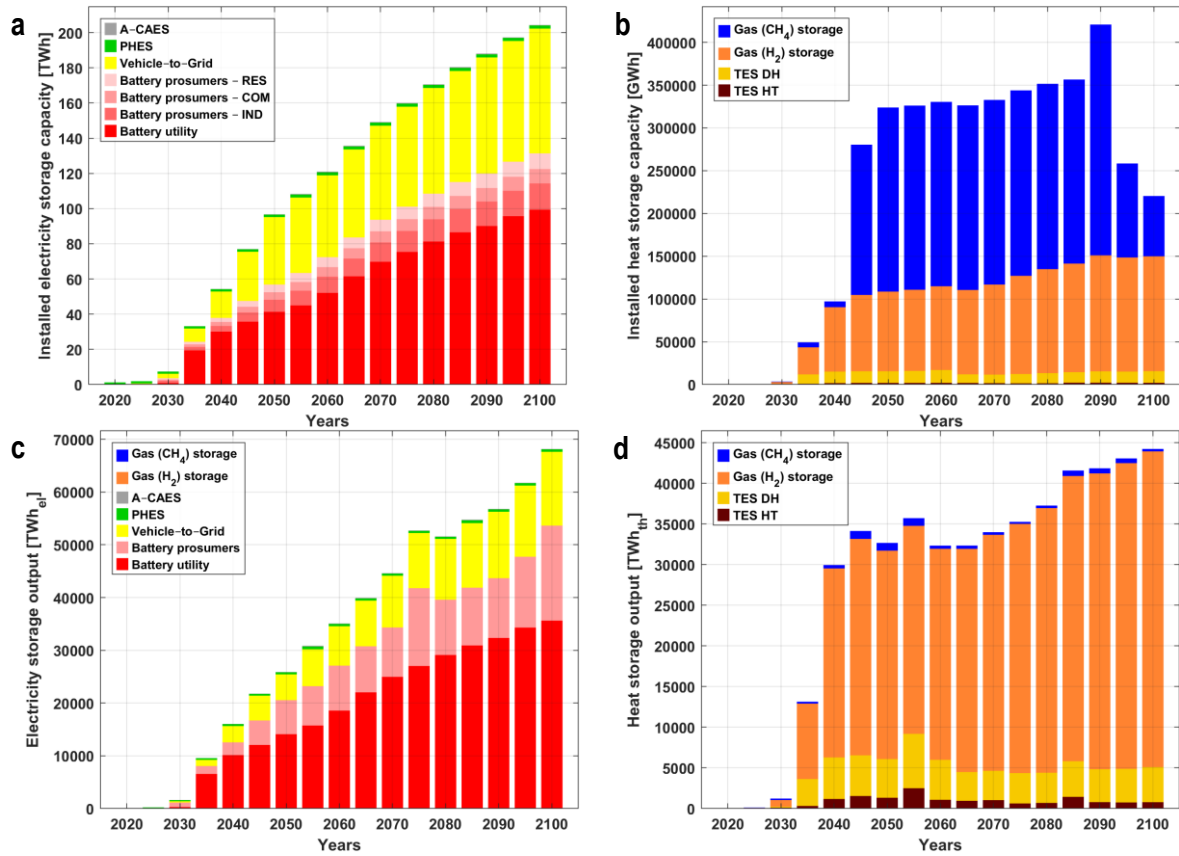


Figure S7. **(a-b)** Global development of installed energy storage capacity for electricity storage **(a)** and heat and gas storage **(b)**. **(c-d)** Global development of energy storage output for electricity including electricity balancing via gas storage output **(c)** and heat and general gas storage output **(d)**.

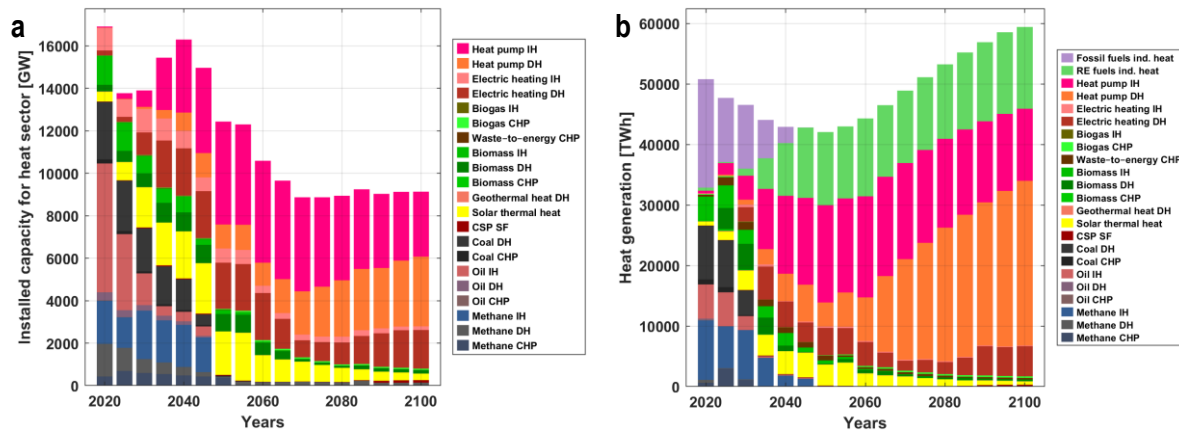


Figure S8. **(a)** Global transition of installed heat generation capacity. **(b)** Global transition of heat generation by technology. Abbreviations: IH – individual heating, DH – district heating, CHP – combined heat and power, CSP SF – concentrated solar thermal power heat collectors with semi-parabolic Fresnel reflector, ind. – industrial (high temperature) heat, RE fuels ind. heat – renewable energy fuels (e-methane, e-hydrogen, biomass/biogas) for industrial heat.

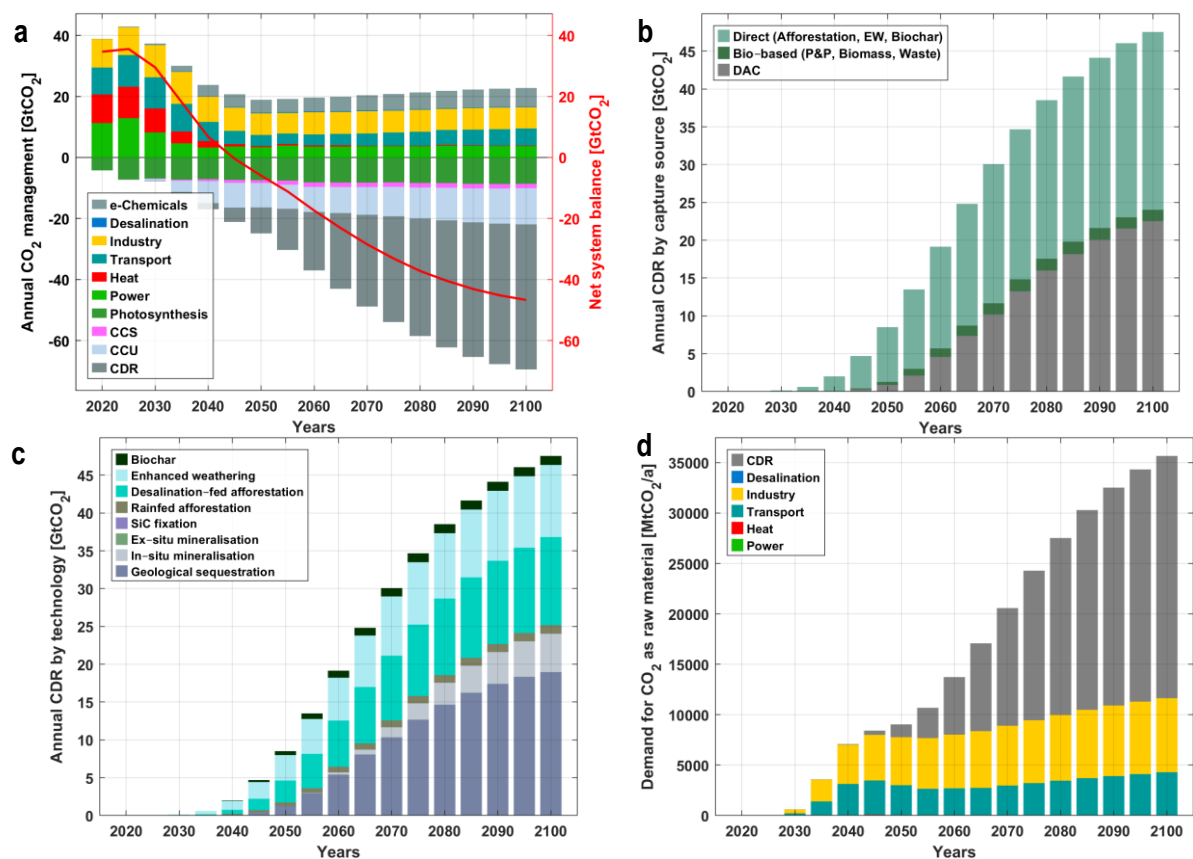


Figure S9. (a) Global development of CO₂ management. (b) Global development of annual CDR by CO₂ source. (c) Global development of annual CDR by technology. (d) Global development of demand for CO₂ as raw material and for CDR. Abbreviations: CCS – carbon capture and sequestration, CCU – carbon capture and utilisation, CDR – carbon dioxide removal, EW – enhanced weathering, P&P – pulp and paper, DAC – direct air capture, SiC – silicon carbide.

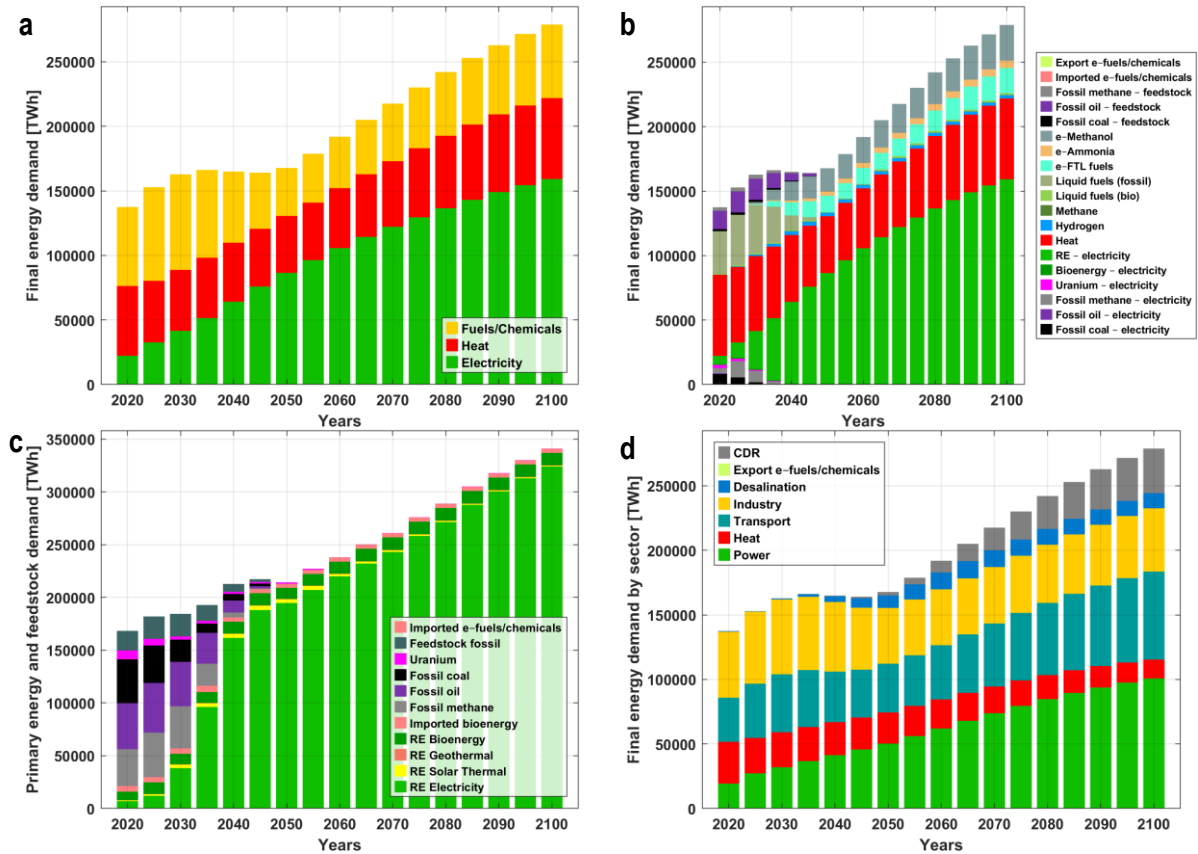


Figure S10. (a) Global development of final energy demand by general energy carrier. (b) Global development of final energy demand by detailed energy carrier. (c) Global development of primary energy and feedstock/non-energy use demand by energy carrier. (d) Global development of primary energy demand by sector. Abbreviations: e-FTL – electricity-based Fischer-Tropsch liquid fuels, RE – renewable energy.

Regional map figures

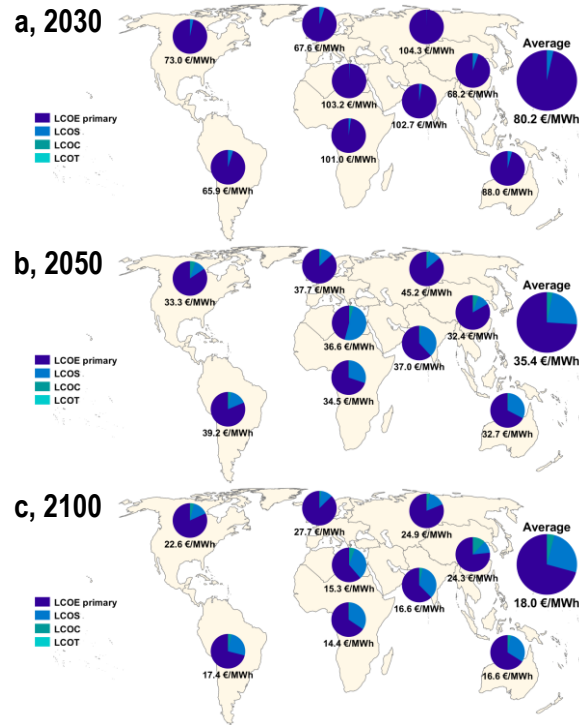


Figure S11. (a-c) Regional structure of levelised cost of electricity in 2030 (a), 2050 (b), and 2100 (c). Abbreviations: LCOE – levelised cost of electricity, LCOS – levelised cost of storage, LCOC – levelised cost of curtailment, LCOT – levelised cost of transmission.

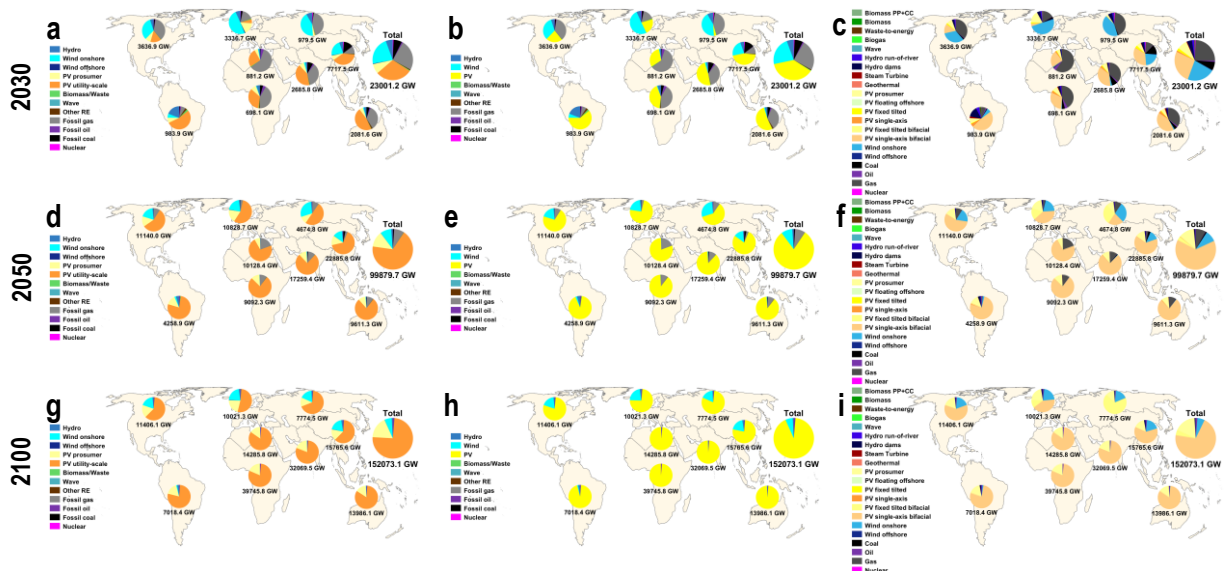


Figure S12. (a-i) Regional structure of electricity generation capacity by technology differentiating prosumer and utility-scale solar PV (a, d, g), no PV differentiation (b, e, h), and full detailed technology portfolio (c, f, i) in 2030 (a, b, c), 2050 (d, e, f), and 2100 (g, h, i).

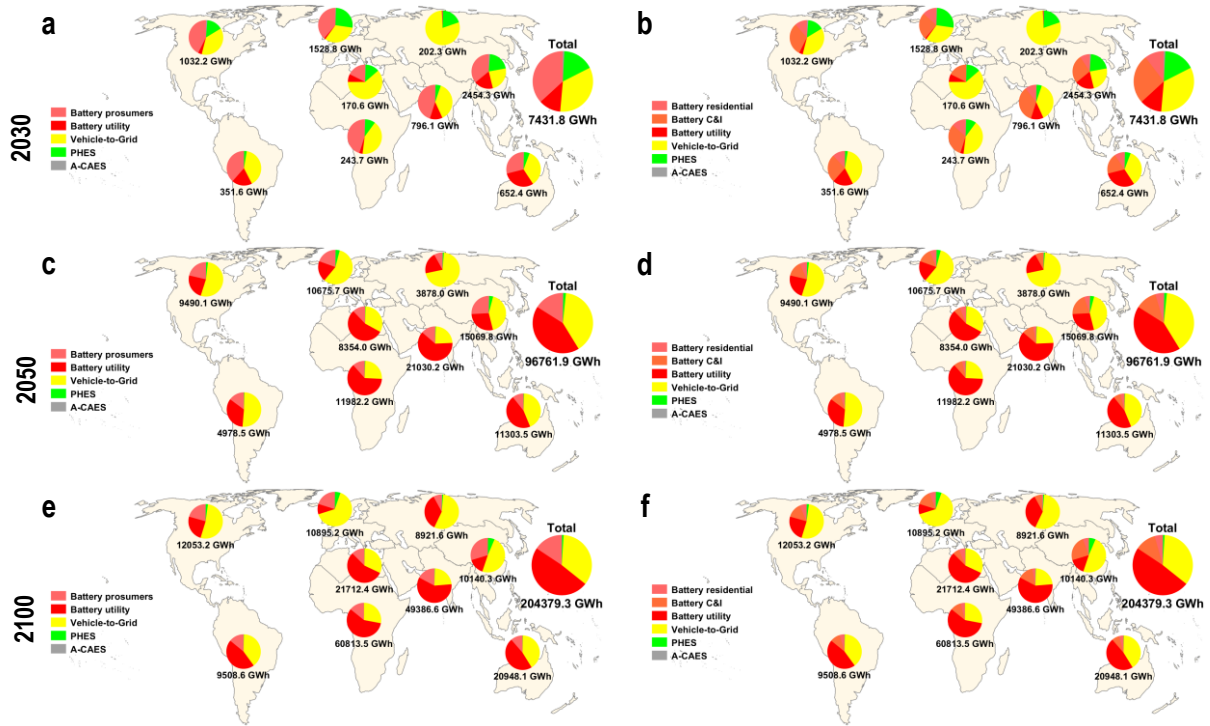


Figure S13. (a-f) Regional electricity storage capacity with aggregated (a, c, e) and differentiated (b, d, f) prosumer batteries in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

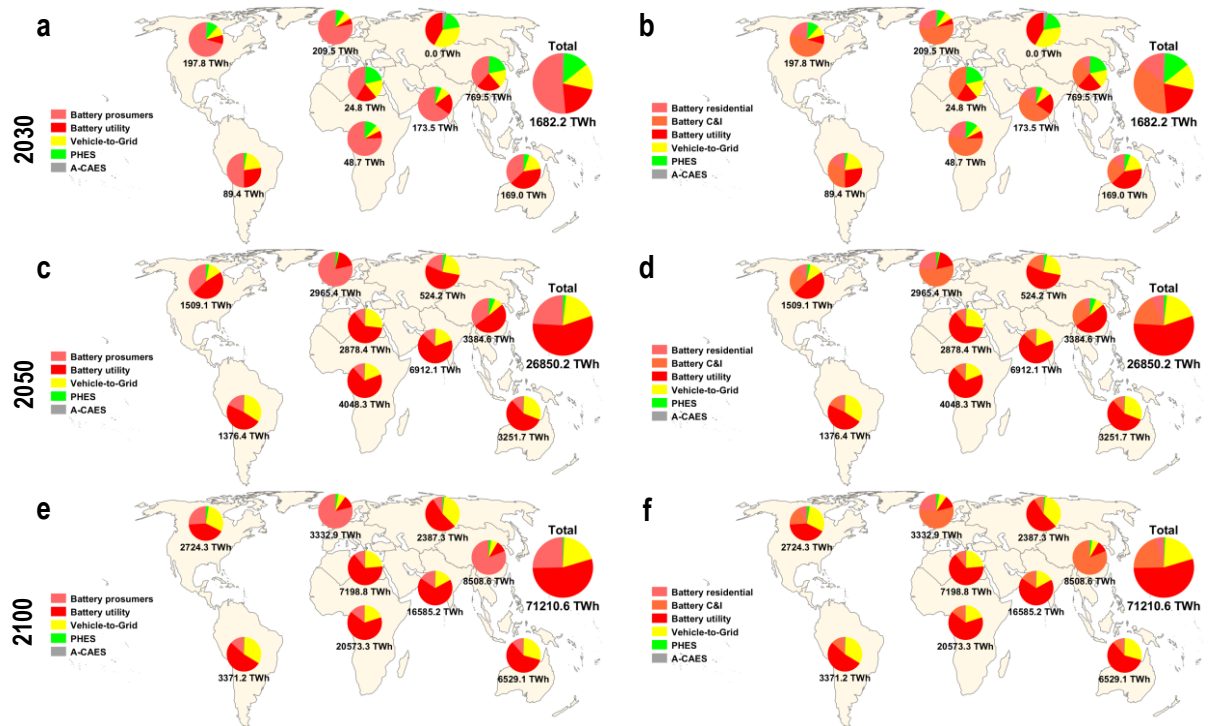


Figure S14. (a-f) Regional electricity storage throughput with aggregated (a, c, e) and differentiated (b, d, f) prosumer batteries in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

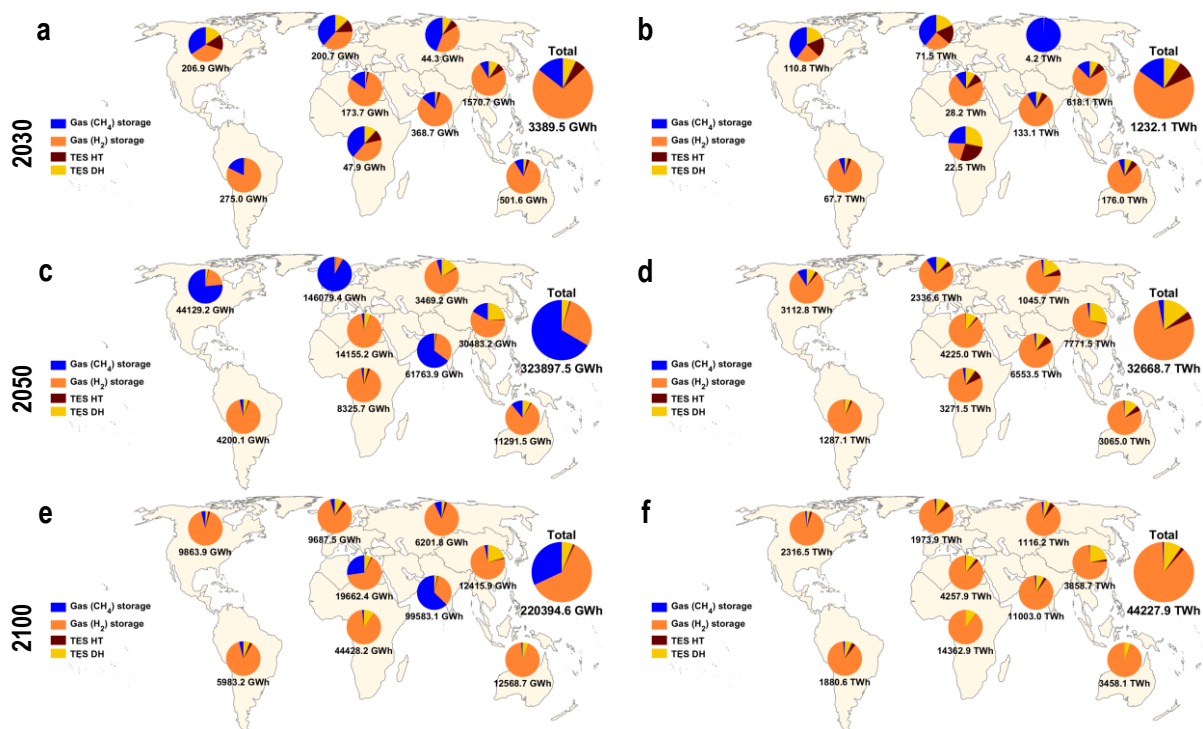


Figure S15. (a-f) Regional heat and gas storage capacity (a, c, e) and energy throughput (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

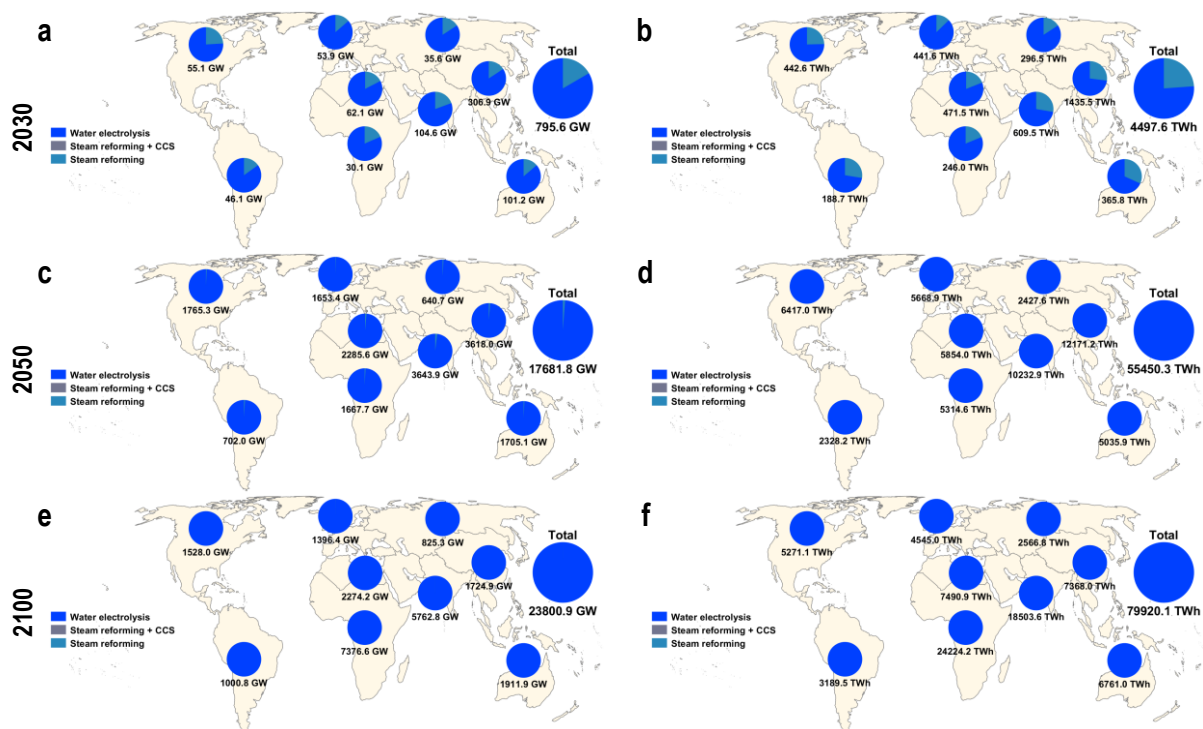


Figure S16. (a-f) Regional hydrogen production capacity (a, c, e) and hydrogen production amount (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

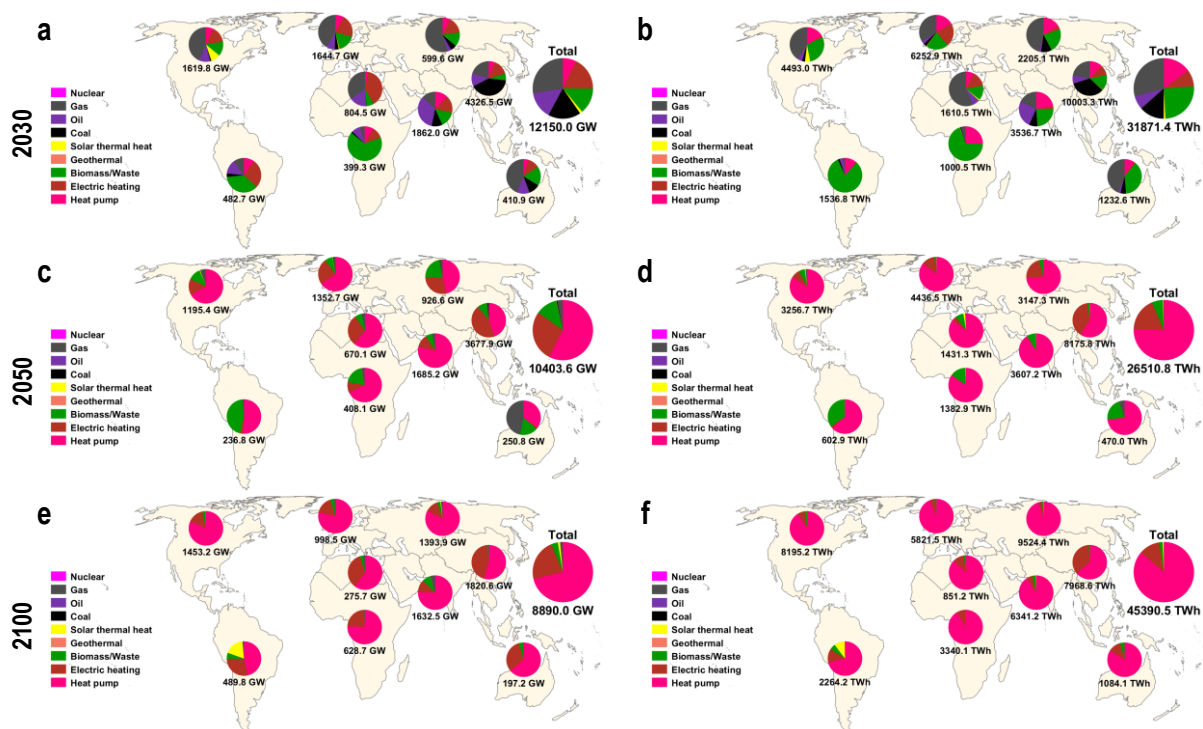


Figure S17. (a-f) Regional installed capacity for heat generation (a, c, e) and heat generation (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

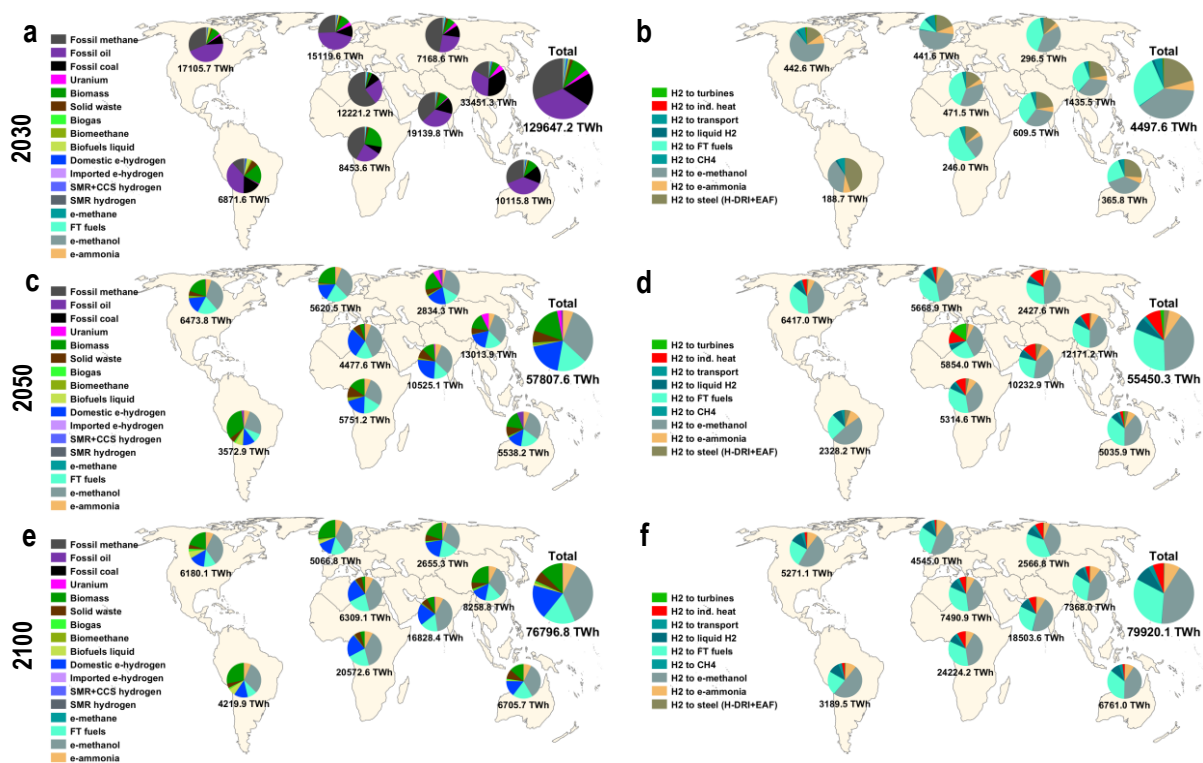


Figure S18. (a-f) Regional supply of fuels and chemicals (a, c, e) and destination of hydrogen (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

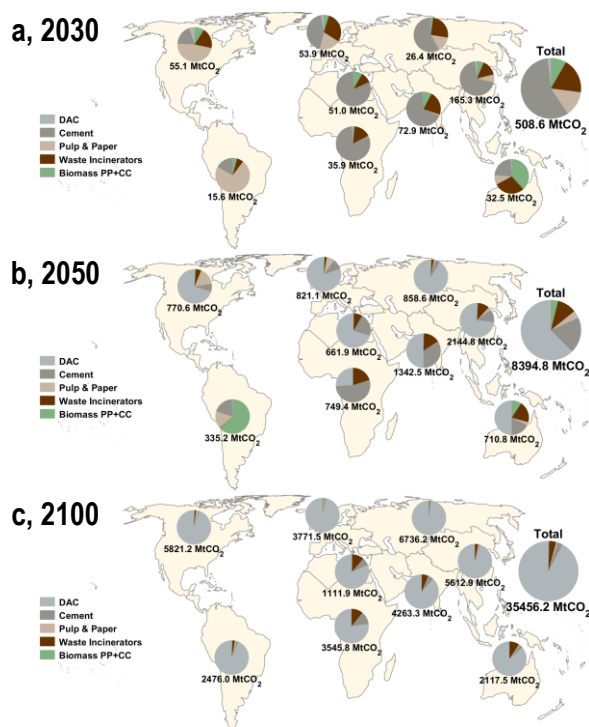


Figure S19. (a-c) Regional structure of CO₂ supply for CCS, CCU, and CDR in 2030 (a), 2050 (b), and 2100 (c).

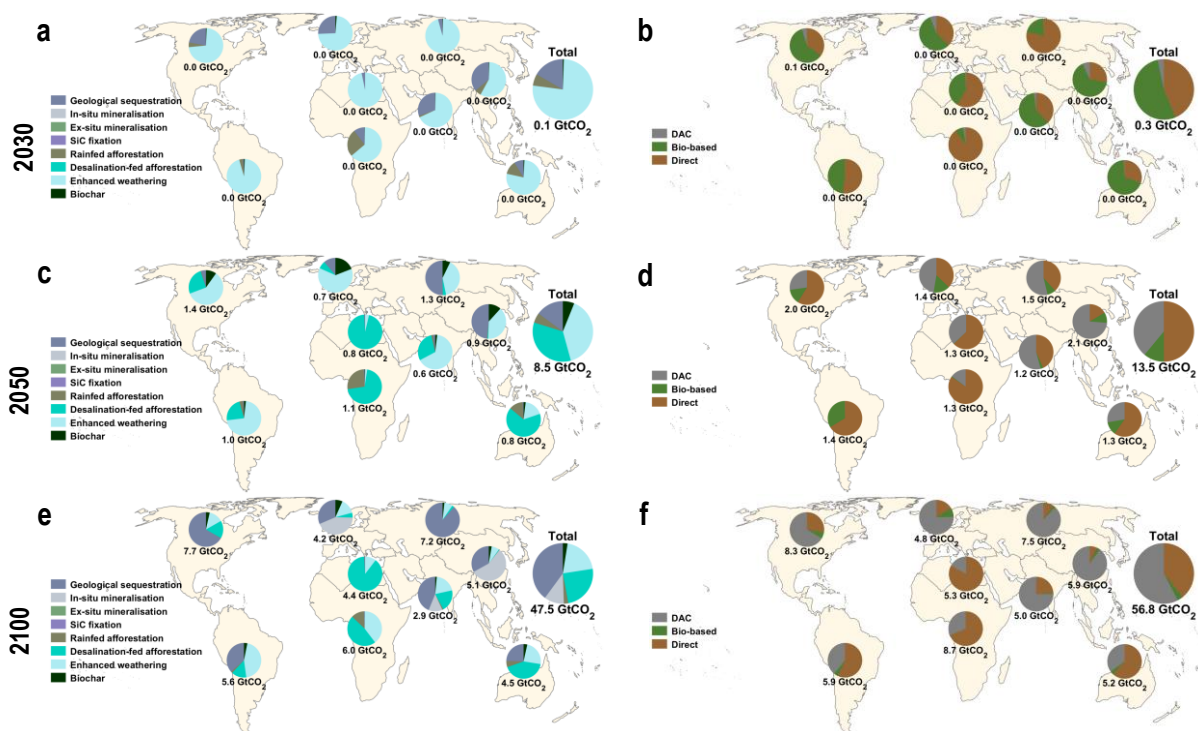


Figure S20. (a-f) Regional structure of CDR by technology (a, c, e) and CDR by CO₂ source (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f). Direct sequestration indicates a direct extraction of CO₂ from the atmosphere without a technical or bio-technical capture process.

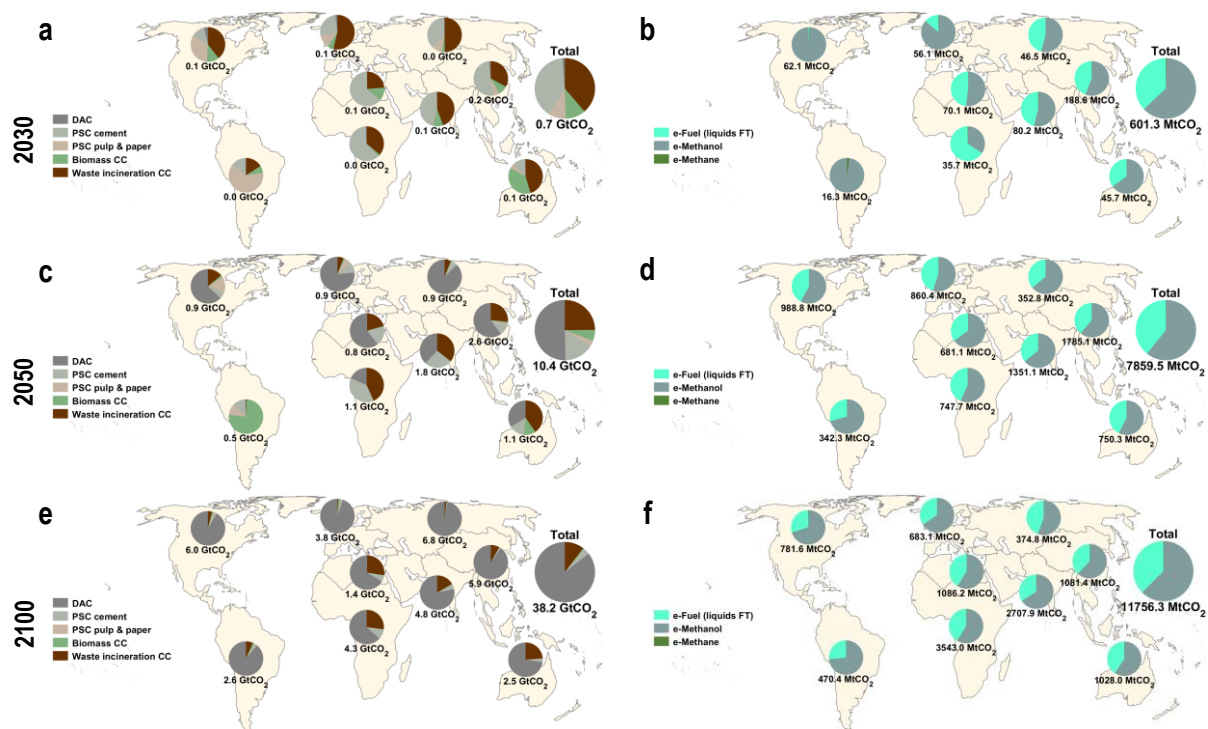


Figure S21. (a-f) Regional structure of CCU by CO₂ source (a, c, e) and by product (b, d, f) in 2030 (a-b), 2050 (c-d), and 2100 (e-f).

1.5°C climate target CO₂ management transition

Figure S22 shows a representative CO₂ management transition for the scenario LEES-1.5-BAL. CO₂ management insignificantly differs between scenarios.

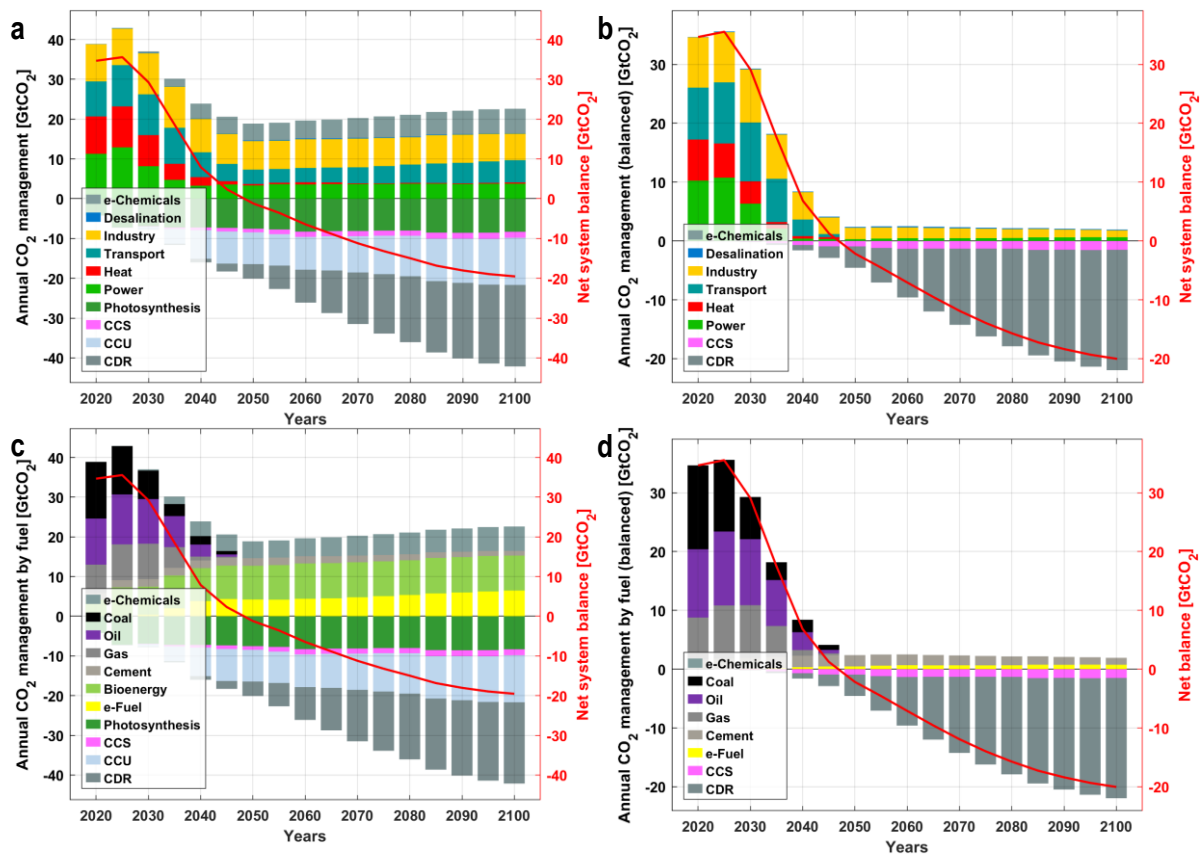


Figure S22. CO₂ management transition for the representative LEES-1.5-BAL scenario. **(a, c)** Unbalanced annual global CO₂ management by type and sector **(a)** and fuel **(c)**. **(b, d)** Balanced annual global CO₂ management by type and sector **(b)** and fuel **(d)**. Balanced CO₂ management eliminates intra-annual circulation (emission and recapture) of CO₂ that directly balances out on an annual basis.

1.0°C climate target CO₂ management transition

Figure S23 shows a representative CO₂ management transition for the scenario LEES-1.0-BAL. CO₂ management insignificantly differs between scenarios.

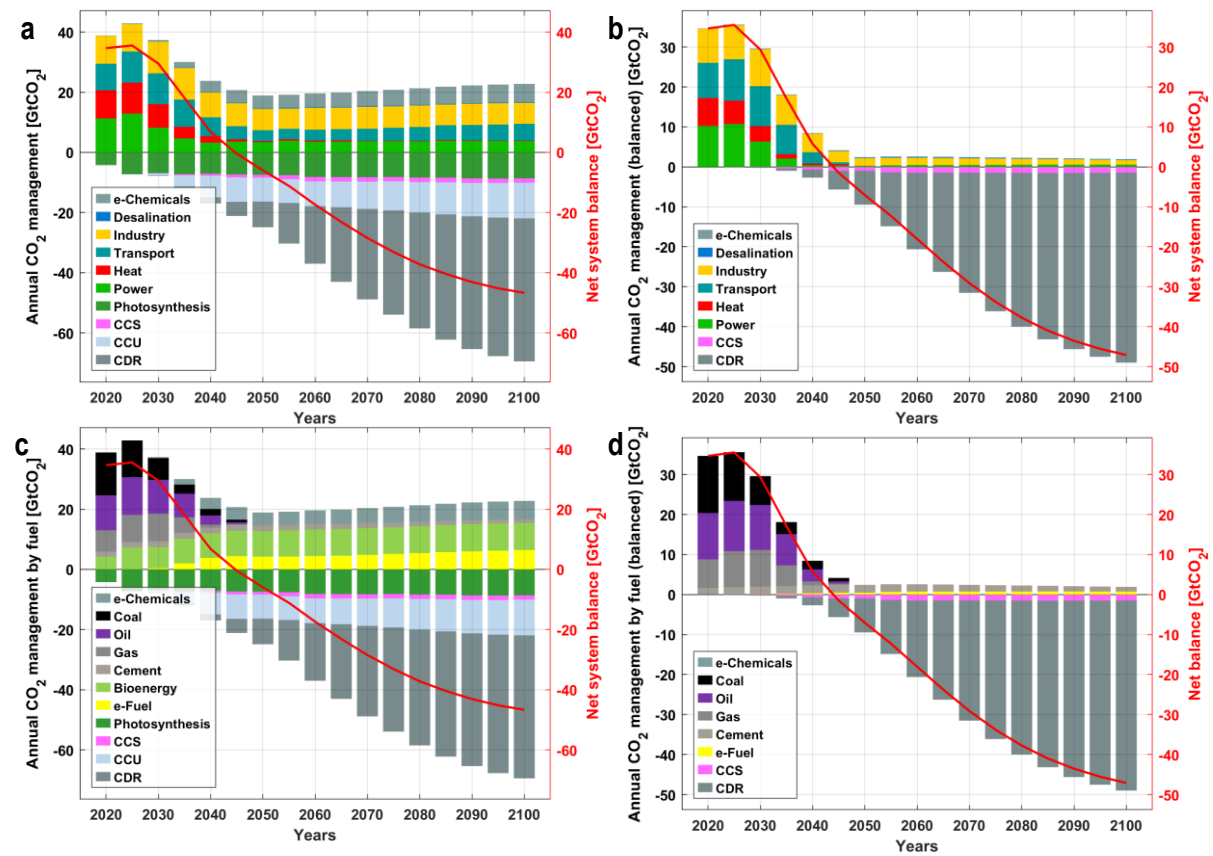


Figure S23. CO₂ management for the representative LEES-1.0-BAL scenario. (a, c) Unbalanced annual global CO₂ management by type and sector (a) and fuel (c). (b, d) Balanced annual global CO₂ management by type and sector (b) and fuel (d). Balanced CO₂ management eliminates intra-annual circulation (emission and recapture) of CO₂ that directly balances out on an annual basis.

Supplementary note 1: Extended literature and scenario review

There is plenty of literature from integrated assessment models (IAM) covering energy system transition and CDR, while planetary boundary compliance is not yet within their scope. As an alternative, scenarios from the AR6 database are analysed regarding their net CO₂ emission balance and climate targets in 2100 to identify the most ambitious scenarios published so far. To do so, data have been extracted from the AR6 database (<https://data.ece.iiasa.ac.at/ar6>) for net CO₂ emissions and global surface air temperature (GSAT) anomaly of the 83.3th percentile (p83) of C1 (limited or no overshoot) and C2 (high overshoot) scenario groups. Figure S24 shows the correlation of net emissions and respective GSAT impact in 5-year steps from 2020 to 2100. The 83.3th percentile has been chosen as it defines the *likely* range in the IPCC AR6 and is chosen to reflect on high confidence levels.

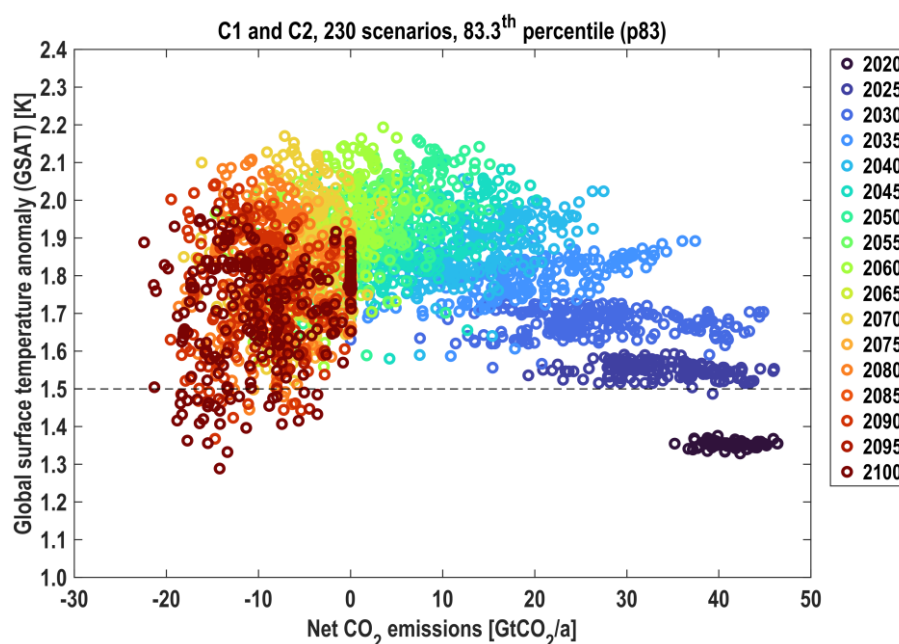


Figure S24. Correlation of net CO₂ emissions and GSAT anomaly of IAM scenarios of the IPCC AR6 database for scenarios with no or limited overshoot (C1) or high overshoot (C2) of 1.5 K from 2020 until 2100. Shown is the p83 of the warming probability, expressing that the GSAT anomaly is likely to stay below the shown values.

Many scenarios result in net-negative CO₂ emissions, while the net-zero threshold is reached in most cases between 2050 and 2060. Of all 230 scenarios, 30 scenarios (13%) among 20 studies and 7 models reach a very high likelihood that the GSAT anomaly stays less than 1.5 K by 2100 (p83). Table S2 gives an overview of these most ambitious scenarios and the associated references according to the database.

Table S2. Overview on studies, C1 and C2 scenarios, and 2100 GSAT anomaly (p83, rounded) of the AR6 scenario database with a 2100 GSAT anomaly of less than 1.5 K. Sorting of the table is done i) by model scenario count, ii) by lowest 2100 GSAT anomaly per source, iii) by 2100 warming level. Single scenario models are sorted alphabetically.

Model	Ref.	Scenario	2100 GSAT anomaly [K]
REMIND/REMIND-MAGPIE	[1]	ADVANCE_2020_1.5C-2100	1.33
		ADVANCE_2030_1.5C-2100	1.36
	[2]	CEMICS-1.5-CDR12	1.40
		CEMICS-1.5-CDR8	1.41
		CEMICS_HotellingConst_1p5	1.41
		CEMICS-1.5-CDR20	1.42
		CEMICS_Linear_1p5	1.47
	[3]	SSP2-19	1.41
		SSP1-19	1.50
	[4]	PEP_1p5C_red_eff	1.42
		PEP_1p5C_full_eff	1.45
		PEP_1p5C_full_NDC	1.46
		PEP_1p5C_full_goodpractice	1.47
	[5]	R2p1_SSP1-PkBudg900	1.45
		R2p1_SSP5-PkBudg900	1.48
	[6,7]	CD-LINKS_NPi2020_400	1.46
		CD-LINKS_INDC2030i_400	1.48
	[8]	SusDev_SSP1-PkBudg900	1.48
		SusDev_SDP-PkBudg1000	1.48
	[9]	CEMICS_SSP1-1p5C-fullCDR	1.49
MESSAGEix-GLOBIOM/MESSAGE-GLOBIOM	[6,7]	CD-LINKS_NPi2020_400	1.36
	[10]	EMF33_1.5C_full	1.44
		EMF33_1.5C_cost100	1.44
	[3]	SSP2-19	1.47
POLES ADVANCE	[1]	ADVANCE_2020_1.5C-2100	1.42
		ADVANCE_2030_1.5C-2100	1.43
C-ROADS	[11]	Ratchet-1.5-limCDR-noOS	1.43
GCAM	[12]	R_MAC_35_n8	1.48
IMAGE	[13,14]	SSP2_SPA2_19I_D	1.45
WITCH-GLOBIOM	[6,7]	CD-LINKS_NPi2020_400	1.29

The most ambitious scenario, CD-LINKS-NPi2020_400, modelled with WITCH-GLOBIOM [6,7] achieves an end-of-century warming of 1.29 K. The scenario achieves this by a strong and stringent reduction of CO₂ emissions by mid-century and scaling net-negative CO₂ emissions to over 14.7 GtCO₂/a by end of the century. However, the scenario also assumes a

significant drop of methane (CH₄) emissions between 2020 and 2025, which limits the overshoot significantly.

The REMIND/REMIND-MagPIE model dominates the available scenarios with warming levels below 1.5 K by 2100. As of the analysis done by Biçakçı et al. [15], the model is leading among IAMs in terms of electrification and share of RE in primary energy. It also leads in hydrogen production from electricity (electrolysis); it requires the least amount of fossil CCS and is one of only three IAMs that consider DACCS.

In other contexts, Streck et al. [16] point to the durability of CDR, often mentioned as one key parameter of CDR. The authors conclude that a portfolio of different CDR options will reduce risks that would occur if relying on a single or only few options. Edelenbosch et al. [17] argue that a maximum emission reduction throughout the entire energy-industry-agriculture system will reduce the need for CDR for a 1.5°C target, though specific challenges and costs may arise. Warszawski et al. [18] analysed scenarios of the IPCC Special Report on 1.5°C (SR1.5) and found that typical scenarios overly rely on CDR for achieving the 1.5°C target and that reasonable scenarios with deep reduction of emissions by 2050 are missing. Merfort et al. [19] conclude that a separation of emission and removal targets favour emission reduction and improve CDR viability. According to Fuhrman et al. [20], CDR portfolio diversification is needed and not yet state-of-the art.

In terms of planetary boundaries, literature on pathway assessments is very scarce. Soergel et al. [21] mention planetary boundaries in the context of sustainable development goals. The presented scenarios, however, are not further assessed if they comply with the planetary boundaries by end of the century. van Vuuren et al. [22] show that IAMs are able to monitor several planetary boundaries, and conclude, that planetary boundaries will largely remain violated by 2050. Scenarios to return within planetary boundaries by 2100 are not presented.

Supplementary note 2: Description of LUT-ESTM

The LUT Energy System Transition Model (LUT-ESTM) [23–26] has integrated all crucial aspects of the power, heat, transport, and industry including desalination sectors into an integrated energy system. Moreover, the model includes prosumers, both power and heat, as part of the energy system. The fundamental approach is shown in Figure S25.

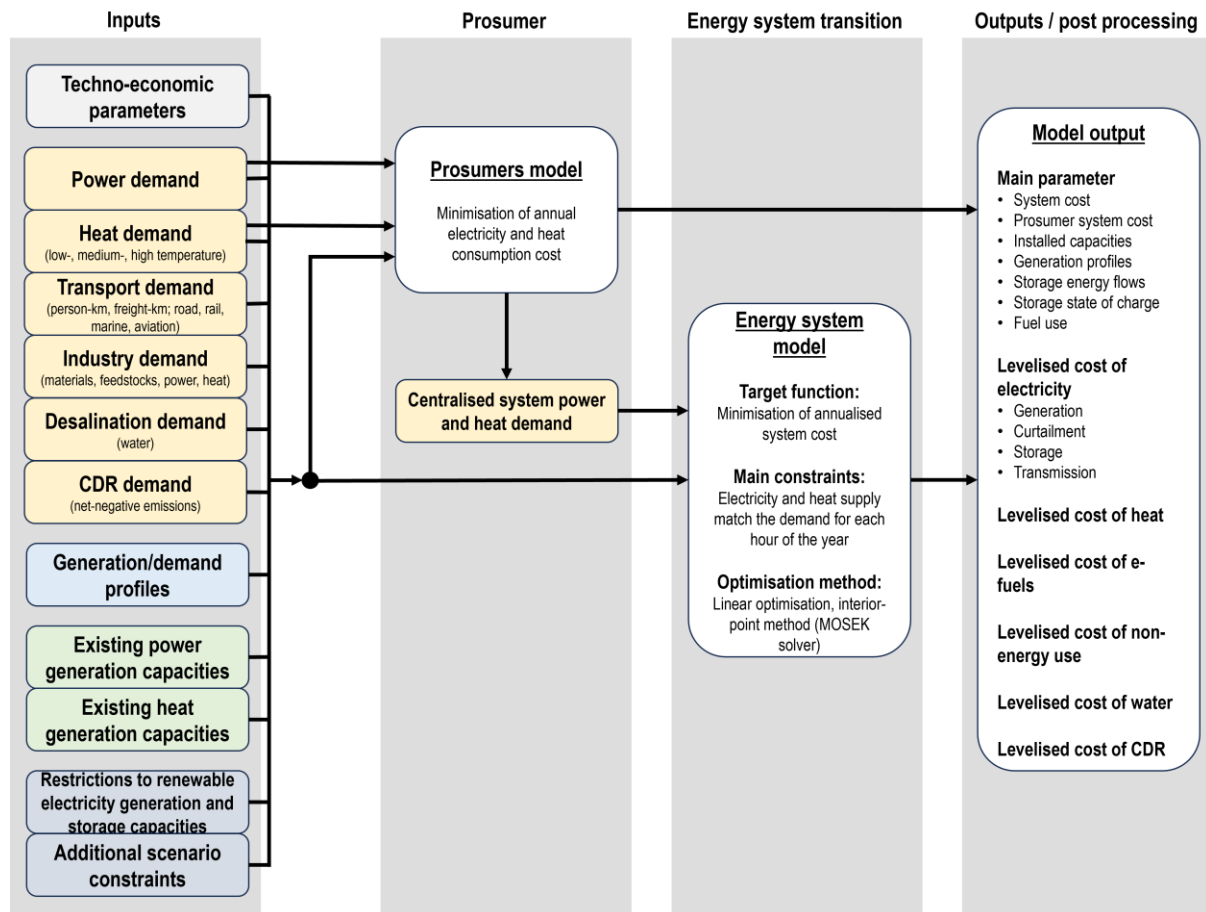


Figure S25. Fundamental structure of LUT-ESTM.

The optimisation model of the energy-industry system is based on a linear optimisation of the system parameters under a set of applied constraints with the assumption of a perfect foresight of renewable energy (RE) supply and energy demand. A multi-node approach enables the description of any desired configuration of sub-regions and power transmission interconnections. The main constraint for the optimisation is the matching of total energy supply and total energy demand values for every hour of the applied year and the optimisation criterion is the minimum of the total annual cost of the system. The hourly resolution of the model significantly increases the computation time. However, it guarantees that for every hour of the year the total supply within a sub-region covers the local demand and enables a more precise system description including synergy effects of different system components.

The optimisation is performed in a third-party solver. Currently, the main option is MOSEK, but other solvers (Gurobi, CPLEX, etc.) can also be used. The model is compiled in the Matlab environment in the LP file format, so that the model can be read by most available solvers.

After the simulation, the results are parsed back to the Matlab data structure and post-processed. A detailed description is provided in Bogdanov et al. [23–26].

Power, heat, transport, and industry including desalination sectors

The model simulates an integrated energy-industry system development under specific given conditions as shown in Figure S26. For each time step, the model defines a cost-optimal energy system structure and operation mode for the given set of constraints: power demand, space and domestic water heating, energy demand for transport, energy and feedstock demand for industry, available electricity generation, energy supply, and storage technologies, financial and technical parameters, and limits on installed capacities for all available technologies. The target of the optimisation is the minimisation of total system cost. The costs of the system are calculated as a sum of the annualised capital expenditures, operational expenditures (including ramping costs), fuel costs, and CO₂ emissions costs for all available technologies. The transition simulation is typically performed for the period from 2020 to 2050 in five-year time intervals.

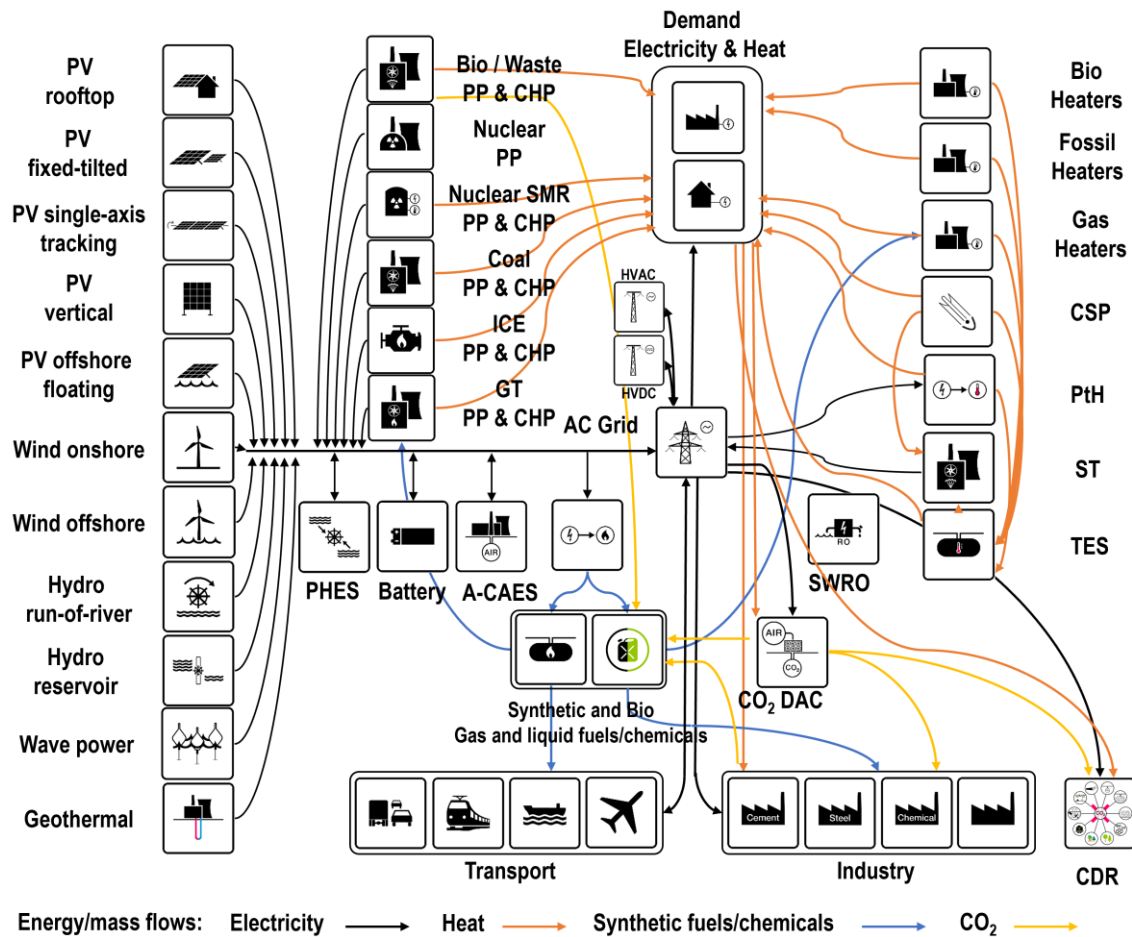


Figure S26. Schematic of LUT-ESTM comprised of energy converters for electricity, heat, fuels, and feedstock, storage technologies, transmission options, and demand sectors [26].

Prosumers

The distributed generation and self-consumption of residential, commercial, and industrial prosumers are included in the energy system analysis and defined with a special model

describing the development of the individual power and heat generation capacities. Prosumers can install their own rooftop PV systems, lithium-ion batteries, buy power from the grid, or sell surplus electricity to fulfil their demand. At the same time, prosumers can install individual heaters for space heating and domestic hot water heating. The target function for prosumers is minimisation of the cost of consumed electricity and heat, calculated as a sum of self-generation equipment annual costs, costs of fuels, and costs of electricity consumed from the grid. The target function of the applied energy model for minimising annual costs is presented in Eq. (S1) and comprises all hours of a year using the abbreviations: generation and storage technologies (t , $tech$), capital expenditures for technology t ($CAPEX_t$), capital recovery factor for technology t (crf_t), fixed operational expenditures for technology t ($OPEXfix_t$), variable operational expenditures technology t ($OPEXvar_t$), installed capacity of technology t ($instCap_t$), annual generation by technology t ($E_{gen,t}$), retail price of electricity ($elCost$), feed-in price of electricity ($elFeedIn$), annual amount of electricity required from the grid (E_{grid}), annual amount of electricity fed-in to the grid (E_{curt}).

$$\min \left(\sum_{t=1}^{tech} (CAPEX_t \cdot crf_t + OPEXfix_t) \cdot instCap_t + OPEXvar_t \cdot E_{gen,t} + elCost \cdot E_{grid} + elFeedIn \cdot E_{curt} \right) \quad (S1)$$

The share of consumers that is expected to be interested in self-generation gradually increases from 9% in 2020 to an in-built limit of 20% by 2050. However, the limit of 20% can be reached earlier than 2050 through the transition depending on the scenario settings and retail electricity prices across the different countries and regions. At least 50% of the self-generated electricity has to be self-consumed and the rest can be sold to the grid at a defined price.

Energy system

The model has integrated all crucial aspects of an energy system. Fossil electricity generation technologies are coal power plants, combined heat and power (CHP), oil-based internal combustion engine (ICE) and CHP, open cycle (OCGT) and combined cycle gas turbines (CCGT), and gas-based CHP. Renewable electricity generation technologies are solar PV (optimally fixed-tilted, single-axis north-south tracking, and rooftop), wind power (onshore and offshore), hydropower (run-of-river and reservoir), geothermal, and bioenergy (solid biomass, biogas, waste-to-energy power plants, and CHP). Fossil heat generation technologies are coal-based district heating, oil-based district and individual scale boilers, and gas-based district and individual scale boilers. RE-based heat generation technologies are concentrated solar thermal power (CSP) parabolic fields, individual solar thermal water heaters, geothermal district heaters, and bioenergy (solid biomass, biogas district heat, and individual boilers).

Storage technologies can be divided into three main categories:

- short-term storage: lithium-ion batteries and pumped hydro energy storage (PHES);
- medium-term storage: adiabatic compressed air energy storage (A-CAES), and high and medium temperature thermal energy storage (TES) technologies;
- long-term gas storage: power-to-gas (PtG: hydrogen, methane) technology, which allows the production of e-hydrogen and e-methane to be utilised in the system.

Sector coupling technologies are power-to-X with e-fuels and e-chemicals (e-hydrogen, e-methane, e-diesel, e-kerosene jet fuel, e-methanol, e-ammonia), steam turbines, electrical heaters, district and individual scale heat pumps, and direct electrical heaters, power-to-mobility including smart charging EV and vehicle-to-grid, and seawater reverse osmosis desalination. These technologies convert energy from one sector into valuable products for another sector to increase total system flexibility, efficiency, and decrease overall costs. A detailed overview can be found in Bogdanov et al. [23–26].

Transportation demand is derived for the modes: road, rail, marine, and aviation for passenger and freight transportation. The road segment is subdivided into passenger light-duty vehicles (LDV), passenger 2/3-wheelers (2W/3W), passenger bus (BUS), freight medium-duty vehicles (MDV), and freight heavy-duty vehicles (HDV). The other transportation modes are comprised of demand for freight and passengers. The demand is estimated in passenger kilometres (p-km) for passenger transportation and in (metric) tonne kilometres (t-km) for freight transportation. Further information and data for transportation demand along with fuel shares and specific energy demand are provided in Khalili et al. [27].

The transportation demand is converted into energy demand by assuming an energy transition from current fuels to fully sustainable fuels by 2050, whereas the following principal fuel types are considered and visualised in Figure S27:

- Road: electricity, hydrogen, liquid fuels;
- Rail: electricity, liquid fuels;
- Marine: electricity, liquid hydrogen, liquid methane, liquid fuels, ammonia, methanol;
- Aviation: electricity, liquid hydrogen, liquid fuels.

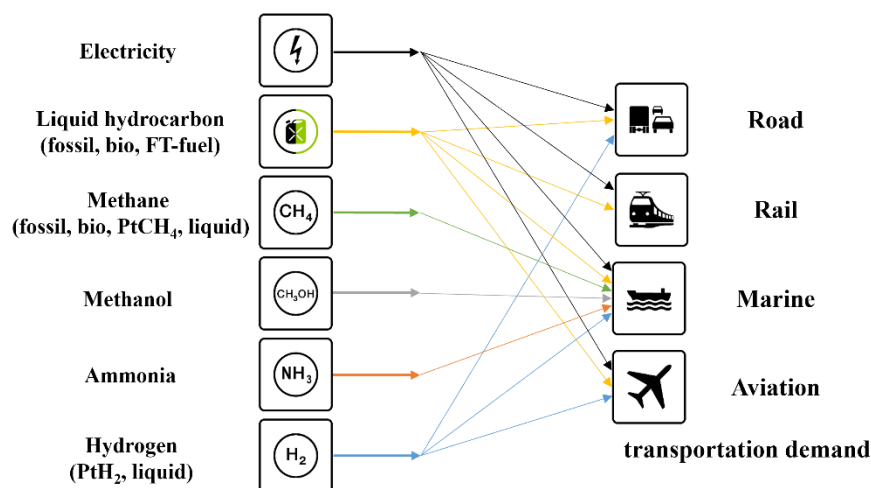


Figure S27. Schematic of the transport modes and corresponding fuels utilised during the energy transition.

The fuel conversion process adopted to produce sustainable e-fuels is shown in Figure S28.

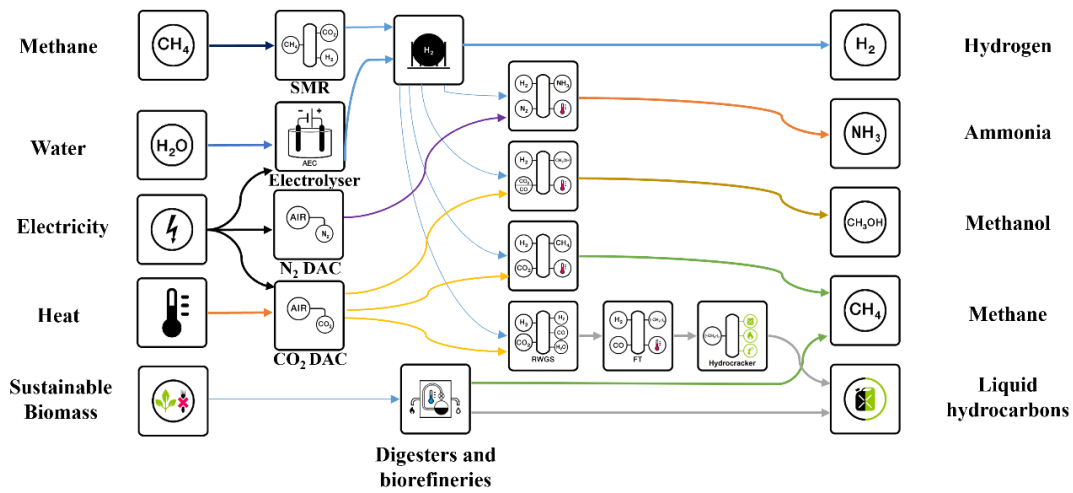


Figure S28. Schematic of the value chain elements in the production of sustainable e-fuels.

The fuel shares of the transportation modes in the road segment are based directly or indirectly on levelised cost of mobility (LCOM) considerations for newly sold vehicles, which change the stock of vehicles according to the lifetime composition of the existing stock. Vehicle stock and overall demand data are then linked to specific energy demand values to calculate demand of fuels and electricity for the transport sector. A more detailed description of the methods is provided in Khalili et al. [27].

Energy balance constraints

The heat sector energy balance is defined by three equations: for industrial high temperature heat demand, for industrial high and medium temperature heat demand, and all centralised heat demand. High temperature heat can only be generated by fuel-based boilers Eq. (S2). Medium temperature heat can also be generated by electrical heating and can be stored in high temperature heat storage and used to produce electricity with steam turbines Eq. (S3). Low temperature heat can also be provided by heat pumps, electric heating rods and waste heat from other technologies Eq. (S4).

$$\forall h \in [1,8760] \sum_t^{techHH} E_{gen,t} \geq E_{demandHH} \quad (S2)$$

$$\forall h \in [1,8760] \sum_t^{techHH} E_{gen,t} + \sum_t^{techMH} E_{gen,t} + E_{stor,disch} \geq E_{demandHH} + E_{demandMH} + E_{stor,ch} \quad (S3)$$

$$\forall h \in [1,8760] \sum_t^{tech} E_{gen,t} + \sum_t^{stor} E_{stor,disch} = E_{demand} + \sum_t^{stor} E_{stor,ch} + E_{curt} + E_{other} \quad (S4)$$

Abbreviations: hours (*h*), technology (*t*), high temperature heat generation technologies (*techHH*), medium temperature heat generation technologies (*techMH*), all heat generation technologies (*tech*), industrial high temperature heat demand ($E_{demandHH}$), industrial medium temperature heat demand ($E_{demandMH}$), total centralised heat demand, including industrial, and space heating and water heating demand (E_{demand}).

Power and heat sector constraints for prosumers have some minor differences. Prosumers can buy electricity from electricity distribution companies (Eq. (S5)). Heating of prosumers based on individual heaters includes fuel, RE and electricity-based heaters, but there is no individual heat storage option (Eq. (S6)).

$$\forall h \in [1, 8760] \sum_t^{tech} E_{gen,t} + \sum_t^{stor} E_{stor,disch} = E_{demand} - E_{grid} + \sum_t^{stor} E_{stor,ch} + E_{curt} + E_{other} \quad (S5)$$

$$\forall h \in [1, 8760] \sum_t^{techIH} E_{genIH,t} = E_{demandIH} + E_{curtIH} \quad (S6)$$

Abbreviations: hours (h), technology (t), all modelled power generation technologies ($tech$), energy generated (E_{gen}), storage technologies ($stor$), energy from discharging storage ($E_{stor,disch}$), energy demand (E_{demand}), electricity energy for charging storage ($E_{stor,ch}$), electricity consumed by heating (E_{other}), excess energy (E_{curt}).

Power and heat generation

The renewable based power and heat generation is defined by historical capacity factors for this technology and the optimal installed capacity of this technology Eq. (S7).

$$\forall h \in [1, 8760] E_{genRE,h} = CF_{genRE,h} \cdot instCap_{genRE} \quad (S7)$$

Abbreviations: hour (h), renewables-based generation technology ($genRE$), energy generated by renewables-based generation technology (E_{genRE}), capacity factor of the technology (CF_{genRE}), installed capacity in the region of the technology ($instCap_{genRE}$).

The fuel-based power and heat generation defined by the optimal installed capacity for this technology Eq. (S8), availability factor for this technology Eq. (S9), this technology used fuel available Eq. (S10), and efficiency of the technology Eq. (S11).

$$\forall h \in [1, 8760] E_{genFU,h} \leq instCap_{genFU} \quad (S8)$$

$$\sum_h^{8760} E_{genFU,h} \leq 8760 \cdot AF_{genFU,h} \cdot instCap_{genFU} \quad (S9)$$

$$\sum_h^{8760} FU_{genFU,h} \leq totalFU_{genFU} \quad (S10)$$

$$\forall h \in [1, 8760] E_{genFU,h} = FU_{genFU,h} \cdot eff_{genFU} \quad (S11)$$

Abbreviations: hour (h), fuel-based generation technology ($genFU$), energy generated by fuel based generation technology (E_{genFU}), installed capacity in the region of the technology ($instCap_{genFU}$), availability factor of the technology (AF_{genFU}), fuel consumption for the hour h ($FU_{genFU,h}$), annual fuel consumption for the hour h ($totalFU_{genFU,h}$), energy conversion efficiency for technology (eff_{genFU}).

For all technologies, capacity is calculated in output units. For cogeneration the capacity is given in electrical units.

For some types of fuel (municipal wastes, industrial biomass wastes, biogas) all available fuel must be consumed for sustainability reasons. Biogas inflow in the system is constant and biogas can be stored only for 48 hours.

The COP for heat pumps can be calculated based on the simplified COP formula derived in Ruhnau et al. [28] as a regression performed for the dataset of COP under different temperature conditions. The formulas for air, water and ground-sourced heat pumps are adopted from Ruhnau et al. [28] and the coefficients are updated based on personal communication with the first author of the paper (Eq. S12-S14).

$$COP_{ASHP} = 6.08 - 0.0941 \cdot \Delta T + 0.000464 \cdot \Delta T^2 \quad (S12)$$

$$COP_{GSHP} = 10.29 - 0.2084 \cdot \Delta T + 0.001322 \cdot \Delta T^2 \quad (S13)$$

$$COP_{WSHP} = 9.99 - 0.2049 \cdot \Delta T + 0.001249 \cdot \Delta T^2 \quad (S14)$$

where *ASHP* is air-sourced HP, *WSHP* water-sourced HP and *GSHP* ground-sourced HP, ΔT is the temperature difference between heat source and sink.

The annual average COP for individual and district heat HPs is calculated based on the sum of space and domestic hot water demand profiles, as described in Eq. (S15).

$$COP_{mean} = \sum_{h=1 \dots 8760} (DHW_h + SHD_h) / \sum_{h=1 \dots 8760} ((DHW_h + SHD_h) / COP_h) \quad (S15)$$

where h is an hour of a year, DHW_h is domestic water heating demand and SHD_h is space heating demand for hour h , COP_h is COP for an hour h .

Power and heat storage

Storage technologies are described as energy storage capacity and storage interface capacity. Energy storage capacity limits the maximum state of charge (SoC) of the storage technology and the amount of energy stored Eq. (S16), while the storage interface capacity limits the maximum power of charge and discharge Eq. (S17), (S18). The energy balance constraint for storage technologies is given in Eq. (S19).

$$\forall h \in [1, 8760] \text{ SoC}_{stor,h} \leq instCapEn_{stor} \quad (S16)$$

$$\forall h \in [1, 8760] E_{stor,ch,h} \leq instCapInt_{stor} \quad (S17)$$

$$\forall h \in [1, 8760] E_{stor,disch,h} \leq instCapInt_{stor} \quad (S18)$$

$$\begin{aligned} \forall h \in [1, 8760] \text{ SoC}_{stor,h} \\ = \text{SoC}_{stor,h-1} \cdot selfDisch_{stor} + E_{stor,ch,h} \cdot eff_{stor,ch} - E_{stor,disch,h} / eff_{stor,disch} \end{aligned} \quad (S19)$$

Abbreviations: hour (h), storage technology ($stor$), storage state of charge for an hour h ($\text{SoC}_{stor,h}$), installed energy capacity of the storage ($instCapEn_{stor}$), installed power capacity of the storage ($instCapInt_{stor}$), charging energy of the storage for an hour h ($E_{stor,ch,h}$), discharging energy of the storage for an hour h ($E_{stor,disch,h}$), hourly self-discharge of the storage ($selfDisch_{stor}$), charge efficiency ($eff_{stor,ch}$), discharge efficiency ($eff_{stor,disch}$).

Power transmission

Power transmission is represented by HVDC and HVAC grids. Each line of the grid is bidirectional, but they are represented in the model as 2 unidirectional lines: import and export. Capacities of import and export lines are equal to the total power capacity of the interconnection, as shown in Eq. (S20). Hourly export/import energy for a sub-region is calculated as the sum of all import lines multiplied by this line transmission efficiency minus the sum of all export line energy flows, as shown in Eq. (S21). The efficiency of energy transmission by HVDC lines depends on the distance and AC/DC converter pair efficiency, as shown in Eq. (S22). The efficiency of energy transmission by HVAC line depends only on distance, as shown in Eq. (S23). For both HVDC and HVAC the distance related losses are calculated in a simplified way.

$$\forall h \in [1,8760] \text{ } line_{import,h} \leq instCap_{line} ; \text{ } line_{export,h} \leq instCap_{line} \quad (S20)$$

$$\forall h \in [1,8760] \text{ } E_{exp/imp,h} = \sum_l^{lines} line_{import,l,h} \cdot eff_l - \sum_l^{lines} line_{export,l,h} \quad (S21)$$

$$eff_l = eff_{cs} \cdot (1 - distance \cdot EffLoss) \quad (S22)$$

$$eff_l = 1 - distance \cdot EffLoss \quad (S23)$$

Abbreviations: hour (h), line (l), energy flow through the power line ($line$), installed capacity of the power line ($instCap_{line}$), exported/imported energy for the region for an hour h ($E_{exp/imp,h}$), total energy import efficiency (eff_i), converter pair efficiency (eff_{cs}), charge length of the line ($distance$), energy loss in the line ($EffLoss$).

The energy transition simulation considers the existing alternating current (AC) power grid of the region, its development trends including direct current (DC) power grids and projected overall electricity transmission and distribution losses according to Sadvovskaia et al. [29].

Transport sector

Transportation demand is expressed in (metric) tonne kilometres (t-km) and passenger kilometres (p-km). Electricity and fuels consumption for each transport mode is calculated based on the transportation demand for this transport mode, share of the vehicles driven with that specific fuel and the specific energy consumption of that transport type for the given fuel (Eq. S24-S29). Power and fuel consumption for a given mix of transportation means is included in the power and fuels (H_2 , diesel, jet fuel, LNG, liquid hydrogen) balance equations on the demand side.

$$\forall h \in [1,8760] \text{ } ElCons_{h,t} = TranspDem_{h,t} \cdot Share_{El} \cdot EffEL_t \quad (S24)$$

$$\sum_h HyCons_{h,t} = \sum_h TranspDem_{h,t} \cdot Share_{Hy} \cdot EffHy_t \quad (S25)$$

$$\sum_h DieselCons_{h,t} = \sum_h TranspDem_{h,t} \cdot Share_{Diesel} \cdot EffDi_t \quad (S26)$$

$$\sum_h JetFuelCons_{h,t} = \sum_h TranspDem_{h,t} \cdot Share_{JetFuel} \cdot EffJF_t \quad (S27)$$

$$\sum_h LNGCons_{h,t} = \sum_h TranspDem_{h,t} \cdot Share_{LNG} \cdot EffLNG_t \quad (S28)$$

$$\sum_h LHyCons_{h,t} = \sum_h TranspDem_{h,t} \cdot Share_{LHy} \cdot EffLHy_t \quad (S29)$$

Abbreviations: hour (h), transport type (t), electricity consumption ($ElCons$), hydrogen consumption ($HyCons$), diesel consumption ($DieselCons$), jet fuel consumption ($JetFuelCons$), LNG consumption ($LNGCons$), liquified hydrogen consumption ($LHyCons$), transportation demand for transport technology t and hour h ($TranspDem_{h,t}$), installed energy capacity of the storage ($instCapEn_{stor}$), installed power capacity of the storage ($instCapInt_{stor}$), share of vehicles driven by specific fuel ($Share$), specific energy consumption of the specific fuel by the transport type t (Eff). Transport types (t) are light-duty vehicles (LDV), buses, 2-3 wheeled transport (2/3W), medium-duty vehicles (MDV), heavy-duty vehicles (HDV), passenger and freight rail, marine, aviation transport.

The functionality of smart charging of EV and V2G in the electric road transportation is defined below. The model delineates the aggregate electricity consumption, available battery capacity, and charging capacity for each road transportation segment and electric vehicle type (BEV or PHEV) by incorporating a range of technical parameters. These parameters include the number of passengers per vehicle, annual mileage, battery capacity, charging capacity, vehicle lifespan, and projected market shares by engine type, all of which are informed by transportation vehicle demand (Eq. S30-S35).

$$totElCons_{mode,y,h} = \sum_{t=BEV,PHEV} ElCons_{seg,t,y} \cdot transpDem_{seg,y,h} \cdot fleetShare_{mode,t,y} \quad (S30)$$

$$fleetShare_{seg,t,y} = numberOfVehicles_{seg,t,y} / \sum_t^{tech} numberOfVehicles_{seg,t,y} \quad (S31)$$

$$numberOfVehicles_{seg,t,y} = \sum_{yy=y-lifetime}^y newVehicles_{seg,t,yy} \quad (S32)$$

$$numberOfVehicles_{seg,t,y} = \frac{(\sum_{h=1}^{8760} transpDem_{seg,y,h})}{milage_{seg,y} \cdot occupancy_{seg,y}} \cdot fleetShare_{seg,t,y} \quad (S33)$$

$$totBatteryCap_{seg,t,y} = \sum_{yy=y-lifetime}^y newVehicles_{seg,t,yy} \cdot batCap_{seg,t,yy} \quad (S34)$$

$$totChargingCap_{seg,t,y} = \sum_{yy=y-lifetime}^y newVehicles_{seg,t,yy} \cdot chargeCap_{seg,t,yy} \quad (S35)$$

where seg – road transportation segment: light-duty vehicle (LDV), BUS, 2/3 wheelers, medium-duty vehicle (MDV), and heavy-duty vehicle (HDV); $tech$, t – technology: BEV, PHEV, FCEV, internal combustion engine (ICE), y – year; h – hour of a year, $lifetime$ – vehicle lifetime; $totElCons$ – total electricity consumed by BEV and PHEV during transportation of passengers and freight; $ElCons$ – specific electricity consumption per passenger km (p-km) or tonne km (t-km); $transpDem$ – transportation demand in p-km or t-km; $fleetShare$ – share of certain transportation technology in the active fleet of vehicles; $numberOfVehicles$ – number of vehicles in the active fleet; $newVehicles$ – new vehicles added to the fleet; $milage$ – annual

milage of an average vehicle, occupancy – average occupancy of a vehicle in passengers or freight tonnes per vehicle; *totBatteryCap* – total battery capacity of the active fleet; *batCap* – battery capacity of an average vehicle; *totChargingCap* – total charging capacity of the active fleet; *chargeCap* – charging capacity of an average vehicle.

The battery capacity and charging capacity can be user-defined and specified on an individual basis for each road transport segment and year of commissioning. The average charging capacity of a vehicle is subsequently calculated from the battery capacity by applying energy-to-power ratio assumptions. By aggregating battery capacity and operation at the fleet level, a significant reduction in computational complexity can be achieved.

Upon determination of the total electricity demand, it is bifurcated into two distinct components: dump charging and smart charging of electric vehicles (Eq. (S36) and (S37)). The dump charging of electric vehicles is governed by a profile that reflects the proportion of grid-connected electric vehicles (as described Eq. (S38)). Conversely, the charging of smart-charged electric vehicles is optimized based on a multifaceted consideration of factors, including the availability of electricity in the grid, discharge profiles resulting from electricity consumption during driving, the state-of-charge of electric vehicle batteries, and the proportion of grid-connected electric vehicles, which collectively define the available charging capacity and battery capacity (see Eq. S39-S44).

$$DumpChCons_{seg,y,h} = dumpChargeShare_{seg,y} \cdot totElCons_{seg,y,h} \quad (S36)$$

$$SmartChCons_{seg,y,h} = (1 - dumpChargeShare_{seg,y}) \cdot totElCons_{seg,y,h} \quad (S37)$$

$$chargeDump_{seg,y,h} = \frac{connectionProfile_{seg,h}}{\sum_{h=1}^{8760} connectionProfile_{seg,h}} \cdot \sum_{h=1}^{8760} DumpChCons_{seg,y,h} \quad (S38)$$

$$\sum_{h=1}^{8760} chargeSmart_{seg,y,h} \geq \sum_{h=1}^{8760} SmartChCons_{seg,y,h} \quad (S39)$$

$$totBatteryCapSmart_{seg,y} = totBatteryCap_{seg,y} \cdot (1 - dumpChargeShare_{seg,y}) \quad (S40)$$

$$totChargingCapSmart_{seg,y} = totChargingCap_{seg,y} \cdot (1 - dumpChargeShare_{seg,y}) \quad (S41)$$

$$chargeSmart_{seg,y,h} \leq totChargingCapSmart_{seg,y} \cdot connectionProfile_{seg,h} \quad (S42)$$

$$\begin{aligned} batterySoC_{seg,y,h} &= (1 - selfDisch_{seg,y}) \cdot batterySoC_{seg,y,h-1} + chargeEff_{seg,y} \\ &\cdot chargeSmart_{seg,y,h} - dischargeSmart_{seg,y,h} / dischargeEff_{seg,y} \end{aligned} \quad (S43)$$

$$batterySoC_{mode,y,h} \leq totBatteryCapSmart_{mode,y} \quad (S44)$$

where *seg* – road transportation segment: LDV, BUS, 2/3 wheeler, MDV, and HDV; *y* – year; *h* - hour of a year; *DumpChCons* – electricity consumption by the dump charged EVs; *dumpChargeShare* – share of the dump charged EVs in the fleet; *SmartChCons* - electricity consumption by the smart charged EV; *connectionProfile* – share of EVs connected to the grid at a certain hour; *chargeDump* – charging profile of dump charging EVs; *chargeSmart* – charging profile of smart charging EVs; *dischargeSmart* – discharge profile of smart charging EVs; *totBatteryCapSmart* – battery capacity of smart charging EVs fleet; *totChargingCapSmart* – charging capacity of smart charging EVs fleet; *batterySoC* –

battery state-of-charge of smart charging EVs fleet; *selfDisch* – self discharge rate of battery per hour; *chargeEff* and *dischargeEff* – charge and discharge efficiency of the battery.

A portion of the battery capacity in smart charged EVs is allocated for V2G operations. The aggregate battery capacity of the V2G-enabled fleet is determined by the proportion of EVs with activated V2G functionality and the corresponding battery volume designated for V2G utilization (Eqs. S45-S48). Furthermore, the available charging and discharging capacity at a given hour is constrained by the proportion of grid-connected EVs (Eq. S49 and S50).

$$totBatteryCapV2G_{seg,y} = totBatterySmart_{seg,y} \cdot shareV2G_{seg,y} \cdot shareBatV2G_{seg,y} \quad (S45)$$

$$totChargingCapV2G_{seg,y} = totChargingCapSmart_{seg,y} \quad (S46)$$

$$batteryV2GSoC_{seg,y,h} \leq totBatteryCapV2G_{seg,y} \quad (S47)$$

$$\begin{aligned} batteryV2GSoC_{seg,y,h} &= (1 - selfDisch_{seg,y}) \cdot batteryV2GSoC_{seg,y,h-1} + chargeEff_{seg,y} \\ &\cdot chargeV2G_{seg,y,h} - dischargeV2G_{seg,y,h} / dischargeEff_{seg,y} \end{aligned} \quad (S48)$$

$$chargeV2G_{eg,y,h} \leq totChargingCapSmart_{eg,y} \cdot connectionProfile_{eg,h} \quad (S49)$$

$$dischargeV2G_{seg,y,h} \leq totChargingCapSmart_{eg,y} \cdot connectionProfile_{eg,h} \quad (S50)$$

where *seg* – road transportation segment: LDV, BUS, 2/3 wheelers, MDV, and HDV; *y* – year; *h* - hour of a year; *totBatteryCapV2G* – battery capacity available for V2G system; *totChargingCapV2G* – charging capacity available for V2G system; *batteryV2GSoC* – battery state-of-charge of V2G system; *chargeV2G* – charging profile of V2G system; *dischargeV2G* – discharge profile of V2G system.

The connection profile serves as a representation of the proportion of vehicles linked to the grid within a given hour, thereby delineating the segment of the fleet capable of charging during that time frame. It is assumed that smart charging vehicles will distribute their charging evenly, with the model exerting control over the charging process. Furthermore, the connection profile delineates the V2G capacity accessible to the system on an hourly basis. This profile is also utilised to estimate the proportion of vehicles in operation and to project the electricity consumption profile of EVs. To account for disparate usage patterns among vehicles, the connection profile is defined separately for each road transport segment, thereby reflecting varying availability for grid services.

The V2G storage capacity is modelled as a subset of the smart charging EV fleet's storage capacity. Consequently, any charging or discharging of V2G storage capacity is accompanied by a corresponding change in the state of charge of the overall smart charging EV batteries (Eqs. (S51) and (S52)). In this formulation, the primary function of the smart charging EV batteries is to serve mobility purposes, with the entire capacity being available for this purpose, even if it necessitates the utilisation of capacity that could otherwise be allocated to V2G applications.

$$dischargeSmart_{seg,y,h} = dischargeV2G_{seg,y,h} + SmartChCons_{seg,y,h} \quad (S51)$$

$$chargeSmart_{seg,y,h} \geq chargeV2G_{eg,y,h} \quad (S52)$$

The smart charging EV's charge and V2G discharge are part of the main electricity supply and demand equation (Eq. (S53)) and on top of charge and discharge losses within EV battery systems the transmission and distribution grid losses within a region are applied to smart charging and V2G.

$$\begin{aligned}
 \sum_g^{gen} elGen_{g,h} + \sum_s^{stor} storDisch_{s,h} + dischargeV2G_{mode,h} + fromGrid_h \\
 = \sum_s^{stor} storCharge_{s,h} + toGrid_h + (1 + T\&DLoss) \\
 \cdot (elDem_h + chargeSmart_{seg,h})
 \end{aligned} \tag{S53}$$

where *seg* – road transportation segment: LDV, BUS, 2/3 wheelers, MDV, and HDV; *gen, g* – electricity generation technologies, *stor, s* – electricity storage technologies, *h* – hour of a year; *elGen* electricity generation in the system; *storDisch* – storage technologies discharge; *dischargeV2G* – V2G system discharge; *elDem* – electricity demand; *storCharge* – storage technologies charging; *chargeSmart* – smart charging vehicles batteries charging; *fromGrid* – electricity from interregional grid; *toGrid* – electricity flow to interregional grid; *T&DLoss* – transmission and distribution grid losses within the region.

Industry system

Industrial processes describe the energy and raw materials demand for cement, steel, chemicals, aluminium, pulp and paper, and desalination. The considered technologies include conventional and improved technology for cement production as detailed in Farfan et al. [30]; conventional (coal-based blast furnace), hydrogen-based direct reduced iron (H-DRI) with electric arc furnace (EAF) and electrowinning of iron (EWIN), steel scrap recycling using EAF for secondary steel production as detailed in Lopez et al. [31]; ammonia, methanol and naphtha production for the chemical industry; alumina and aluminium production, aluminium recycling for secondary aluminium production; pulp and paper mills for paper production; seawater desalination covers seawater reverse osmosis (SWRO), multi stage flash (MSF) desalination and multi effect distillation (MED) according to Caldera and Breyer [32]. Other industry is considered to be supplied with industrial process heat, mainly based on conventional fuels in the initial periods of the transition, which shifts towards high shares of direct electric heat supply, some bioenergy, and hydrogen-based heat supply in the later periods.

For each industrial product the model traces the electricity, heat, fuels and raw materials consumption, and the excess heat generation for some technologies. Electricity, heat, and fuels consumption flows are included to the power, heat and fuels balancing equations on demand side, heat flows are separated into three flows: high, medium and low temperature heat and balanced accordingly.

$$\forall h \in [1,8760] \ ElCons_{h,t} = ProductOutput_{h,t} \cdot EffEL_t \tag{S54}$$

$$\forall h \in [1,8760] \ HeCons_{h,t} = ProductOutput_{h,t} \cdot EffHe_t \tag{S55}$$

$$\forall h \in [1,8760] \text{ RawMaterial}_{h,t,RM} = \text{ProductOutput}_{h,t} \cdot \text{EffRM}_{t,RM} \quad (\text{S56})$$

$$\forall h \in [1,8760] \text{ HeOutput}_{h,t} = \text{ProductOutput}_{h,t} \cdot \text{HeReq}_t \quad (\text{S57})$$

Abbreviations: hour (h), industry technology (t), raw material (RM), industry (t) products output (ProductOutput_t), electricity consumption (ElCons), heat consumption (HeCons), raw material RM consumption ($\text{RawMatherial}_{h,t,RM}$), heat output (HeOutput), electricity consumption per unit of industry (t) production output (EffEl), electricity consumption per unit of industry (t) production output (EffEl_t), heat consumption per unit of industry (t) production output (EffHe_t), raw material RM consumption per unit of industry (t) production output ($\text{EffRM}_{t,RM}$), recovered heat per unit of industry (t) production output (EffHe_t). Industry technologies (t) are steel: oxygen blast furnace (BF-BOF), electric arc furnace steel recycling (EAF), hydrogen direct reduced iron (H-DRI), electrowinning process (EWIN); cement: business-as-usual (BAU) and improved process, alumina production, aluminium: primary aluminium production and recycling; pulp and paper; water electrolysis, steam reforming, steam reforming with carbon capture, CO₂ direct air capture, CO₂ point source capture for P&P industry, CO₂ point source capture for cement industry, methanation, liquefaction of H₂, liquefaction of CH₄, Fischer-Tropsch synthesis, ammonia and methanol production, Raw materials (RM) are iron ore (steel industry), limestone (cement and alumina industry), hard coal (blast furnace steel production), charcoal (other steel), scrap iron (steel industry), hydrogen (hydrogen direct reduced iron, e-fuels and chemicals production), bauxite (alumina production), sodium hydroxide (alumina production), alumina (aluminium production), aluminium scrap (aluminium recycling), wood (pulp and paper industry), methane (steam reforming, fossil based chemical industry), CO₂ (methanol and e-fuels production).

e-Fuels, ammonia, and methanol production is fully optimised by the model, and the model defines the optimal capacity of the production units and hourly operation (Eq. (S58)), and availability factors are set to 95% (Eq. (S59)). Fischer-Tropsch, methanation and LNG units operate at baseload (Eq. (S60)). For cement, steel, aluminium, alumina, pulp and paper industry system only optimises the production, raw materials and energy consumption profiles, and capacity capital expenditures for these industries are not included in the model. However, some flexibility is still allowed for these technologies, as the minimum FLh are set to 4000 h (Eq. (S61)).

$$\forall h \in [1,8760] E_{outPtX,h} \leq instCap_{PtX} \quad (\text{S58})$$

$$\sum_h^{8760} E_{outPtX,h} \leq 8760 \cdot AF_{PtX,h} \cdot instCap_{PtX} \quad (\text{S59})$$

$$\forall h \in [1,8760] E_{out BL_PtX,h} = AF_{PtX,h} \cdot instCap_{BL_PtX} \quad (\text{S60})$$

$$\max_h P_{Ind,h} \cdot 4000 \leq \sum_h^{8760} P_{Ind,h} \quad (\text{S61})$$

Abbreviations: hour (h), e-fuels and synthetic chemical production technology (PtX), baseload e-fuels production technology (BL_PtX), other industry technology (Ind), e-fuels and synthetic chemicals produced (E_{outPtX}), other industrial products output (P_{Ind}), installed capacity in the region of the technology ($instCap$), availability factor of the technology (AF). Enabled e-fuels and synthetic chemical PtX technologies are water electrolysis, steam reforming, CO₂ direct air capture, methanation, liquefaction of H₂, liquefaction of CH₄, Fischer-Tropsch, ammonia and methanol.

CDR system

CDR modelling is similar to industrial processes and describes the energy and raw materials demand for various CDR technologies. Depending on technology the model calculates energy demand in form of electricity or heat, and raw materials demand (CO₂, biomass, specific minerals, and/or water) for respective CO₂ volumes requested. Most technologies require captured CO₂ as the key input, with exception of desalination, enhanced weathering and biochar technologies, which perform direct sequestration from the atmosphere. Electricity, heat, biomass, and water consumption flows are included to the power, heat, fuels and desalinated water balancing equations on the demand side.

$$\forall h \in [1,8760] \text{ } ElCons_{h,t} = CO2Seq_{h,t} \cdot EffEL_t \quad (S62)$$

$$\forall h \in [1,8760] \text{ } HeCons_{h,t} = CO2Seq_{h,t} \cdot EffHe_t \quad (S63)$$

$$\forall h \in [1,8760] \text{ } RawMaterial_{h,t,RM} = CO2Seq_{h,t} \cdot EffRM_{t,RM} \quad (S64)$$

Abbreviations: hour (h), CDR technology (t), raw material (RM), CDR type (t) sequestration volume ($CO2Seq_t$), electricity consumption ($ElCons$), heat consumption ($HeCons$), raw material RM consumption ($RawMaterial_{h,t,RM}$), electricity consumption per unit of CO₂ sequestered ($EffEL_t$), heat consumption per unit of CO₂ sequestered ($EffHe_t$), raw material RM consumption per unit of CO₂ sequestered ($EffRM_{t,RM}$).

CDR balance equations define total annual sequestration as total volume of CO₂ sequestered by all technologies, which should exceed annual CDR demand and volume of CO₂ captured at unsustainable point sources.

$$\sum_{h=1}^{8760} \sum_t^{tech} CO2Seq_{h,t} \geq CDR_{demand} + \sum_{h=1}^{8760} \sum_{tc}^{unsustPSC} CO2Capt_{h,tc} \quad (S65)$$

Abbreviations: hour (h), CDR technology ($t, tech$), unsustainable CO₂ point source capture technology ($tc, unsustPSC$), CDR type (t) sequestration volume ($CO2Seq_t$), unsustainable point source technology (t) CO₂ captured ($CO2Capt_{tc}$), annual CDR demand (CDR_{demand}).

Figure S29 shows the electricity, heat, biomass, water, and CO₂ flows of the CDR sector.

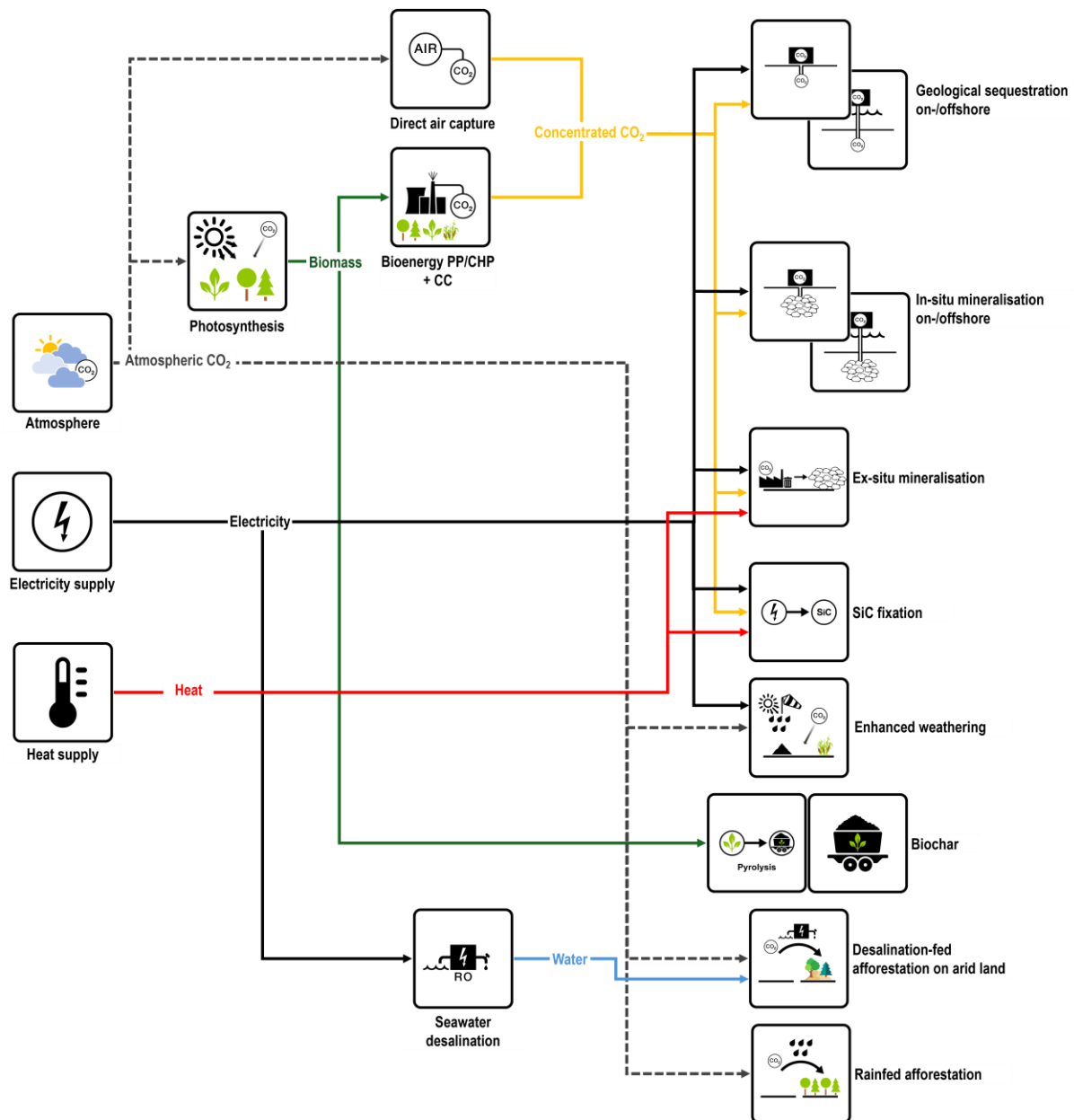


Figure S29. Schematic of the CDR sector CO₂ and energy flows. Abbreviations: PP/CHP + CC – power plants/combined heat and power with carbon capture, SiC – silicon carbide.

Unsustainable CO₂ point source capture technologies normally include thermal power plants running on fossil fuels and steam methane reforming units with carbon capture, but depending on scenario may also include waste incinerators with carbon capture or point source capture at cement production units.

Capacity definition through transition periods and system cost calculation

The active capacity existing in the system is defined at each of the steps for each of the regions based on the data of the capacity installed at previous steps and the lifetime for the given technology at given commissioning year as presented in Eq. (S66).

$$\forall t \in [tech] \text{ existingCap}_{t,year} = \sum_{y=1960}^{year-5} \text{newCap}_{t,y} \cdot ((y + N_{t,y}) > year) \quad (S66)$$

Abbreviations: year (y , $year$), generation and storage technologies (t , $tech$), existing active capacity for technology t at the modelled year ($\text{existingCap}_{t,year}$), new built capacity for technology t at the previous year y ($\text{newCap}_{t,y}$), lifetime of the capacity of technology t built at year y ($N_{t,y}$).

Then, the model optimisation results in the optimal regional capacity of the technologies in the given year, which defines the new built capacity needed by the system as defined in Eq. (S67).

$$\forall t \in [tech] \text{ newCap}_{t,year} = \text{instCap}_{t,year} - \text{existingCap}_{t,year} \quad (S67)$$

Abbreviations: modelling year ($year$), generation and storage technologies (t , $tech$), existing active capacity for technology t at the modelled year ($\text{existingCap}_{t,year}$), new built capacity for technology t at the previous year y ($\text{newCap}_{t,y}$), total capacity for technology t at given year $year$ as defined by the model optimisation ($\text{instCap}_{t,year}$).

The energy costs calculations in the post processing phase are based on a historical approach, where the annualised cost of the system considers the financial assumptions in the periods when these capacities were built, unlike the approach used in the optimisation. For the variable opex calculations, the energy output of technologies is split accordingly to the capacity age structure as defined in Eq. (S68).

$$\forall t \in [tech], \forall y \in [1960 \dots year] E_{genSplit,t,y} = E_{gen,t,year} \cdot \left(\text{newCap}_{t,y} \cdot ((y + N_{t,y}) > year) \right) / \text{instCap}_{t,year} \quad (S68)$$

Abbreviations: modelling year ($year$), all years from 1960 (y), generation and storage technologies (t , $tech$), annual generation by technology t by capacity built at year y ($E_{genSplit,t,y}$), new built capacity for technology t built at year y ($\text{newCap}_{t,y}$), annual generation by technology t defined by the model for the modelling year $year$ ($E_{gen,t,year}$), total capacity for technology t at given year $year$ as defined by the model optimisation ($\text{instCap}_{t,y}$), lifetime of the capacity of technology t built at year y ($N_{t,y}$).

Then the annualised cost of the system at the given year is calculated accordingly to the Eq. (S69).

$$\begin{aligned} \text{annualCost}_{year} = & \sum_{r=1}^{reg} \sum_{t=1}^{tech} \sum_{y=1960}^{year} (CAPEX_{r,t,y} \cdot crf_{r,t,y} + OPEXfix_{r,t,y}) \\ & \cdot \left(\text{newCap}_{r,t,y} \cdot ((y + N_{t,y}) > year) \right) + OPEXvar_{r,t,y} \cdot E_{genSplit,r,t,y} \\ & + \text{rampCost}_t \cdot \text{totRamp}_{r,t} \end{aligned} \quad (S69)$$

This historical cost calculation approach is used for other cost calculations including LCOE and split of LCOE in sub-categories. Abbreviations: modelling year ($year$), all years from 1960 (y), generation and storage technologies (t , $tech$), capital expenditures for technology t in region

r and year y ($CAPEX_{r,t,y}$), capital recovery factor for technology t in region r and year y ($crf_{r,t,y}$), fixed operational expenditures for technology t in region r and year y ($OPEXfix_{r,t,y}$), variable operational expenditures technology t in region r and year y ($OPEXvar_{r,t,y}$), new built capacity for technology t built in region r at year y ($newCap_{r,t,y}$), lifetime of the capacity of technology t built at year y ($N_{t,y}$), annual generation by technology t in region r at year $year$ by capacity built at year y ($E_{genSplit,r,t,y}$), cost of ramping of technology t ($rampCost_t$), sum of power ramping values during the year for the technology t in the region r ($totRamp_{r,t}$).

Results preparation and cost calculations

All optimisation results are collected and converted from the solver output form to the MATLAB structure. This structure contains all information about the system: installed capacities of all system elements, its operation modes, energy, fuel and other product flows.

The data on the structure and operation of the energy system in combination with financial and technical assumptions give a full description of the system. Based on these numbers, the annual costs of each component and the whole system, costs to specific sectors, costs of products (electricity, heat, synthetic fuels, water), and different components of these costs (primary generation, storage, transmission, curtailment components of electricity prices etc.) can be calculated.

The total annualised cost of the system is calculated as the sum of all sectors costs Eq. (S70), which includes annualised capital expenditures and operational expenditures of all system elements Eq. (S71):

$$totalCost_{sys} = elSysCost + elProsCost + heatSysCost + heatIndCost + transpSysCost + industrSysCost \quad (S70)$$

$$totalCost_{sys} = \sum_{t=1}^{tech} (CAPEX_t \cdot crf_t + OPEXfix_t) \cdot Cap_t + OPEXvar_t \cdot E_{gen,t} \quad (S71)$$

$$crf_{r,t,y} = \frac{WACC_{r,t,y} \cdot (1 + WACC_{r,t,y})^{N_{t,y}}}{(1 + WACC_{r,t,y})^{N_{t,y}} - 1} \quad (S72)$$

Abbreviations: total annualised cost of the system ($totalCost_{sys}$), annualised cost of the centralised power sector ($elSysCost$), annualised cost of the electricity prosumers sector ($elProsCost$), annualised cost of the centralised heat sector ($heatSysCost$), annualised cost of the individual heat sector ($heatIndCost$), annualised cost of the transport sector ($transpSysCost$), annualised cost of the industry sector ($industrSysCost$), all technologies ($tech$), technology (t), capital expenditures ($CAPEX$), capital recovery factor for technology t (crf_t), annual fixed operational expenditures ($OPEXfix$), variable operational expenditures ($OPEXvar$), installed capacity of the technology t (Cap_t), annual output for the technology t ($E_{gen,t}$), weighted average cost of capital for technology t in region r and year y ($WACC_{t,r,y}$), lifetime for technology t and year y ($N_{t,y}$).

Total levelised cost of electricity in the system ($LCOE_{total}$) is calculated as the electricity demand weighted average of the centralised power system LCOE ($LCOE_{sys}$) and prosumers sector LCOE ($LCOE_{pros}$); the formula is presented in Eq. (S73). The centralised power system LCOE ($LCOE_{sys}$) is comprised of levelised cost of consumed electricity ($LCOE_{prim}$), levelised cost of storage ($LCOS$), levelised cost of curtailed electricity ($LCOC$), levelised cost of electricity transition ($LCOT$) and levelised cost of prosumer feed-in reimbursement

(*LCOFS*) as summarised in Eq. (S74). For the prosumer sector, the total LCOE (*LCOEpros*) is comprised of the levelised cost of consumed electricity (*LCOEprim*), levelised cost of storage (*LCOS*), and levelised cost of prosumer feed-in reimbursement (*LCOFS*) as presented in Eq. (S75). Levelised cost of generated electricity is calculated as the total annualised cost of the electricity generation system divided by total annual generation according to Eq. (S76).

In these calculations operational expenditures include costs of fuel and GHG emissions cost per unit of generated electricity. The electricity generation systems also include parts of the fuel production facilities, which are used for fuel production for power system generators. Levelised cost of consumed electricity is calculated based on the cost of the generated electricity (*LCOEgen*), excluding electricity lost due to curtailment, storage and transmission system losses according to Eq. (S77). Levelised cost of storage is calculated as the annualised cost of storage system equipment and annual cost of electricity losses divided by total electricity consumption according to Eq. (S78). Storage systems also include parts of the fuel production facilities, which are used for fuel production for the storage system generators (e.g. for Power-to-Gas – Gas-to-Power). Levelised cost of curtailment is calculated as the annual cost of curtailed electricity divided by total electricity consumption according to Eq. (S79). Levelised cost of transmission is the calculated area total annualised cost of power grid capacity and annual cost of electricity losses divided by total electricity consumption, and multiplied by regional grid utilisation weights according to Eq. (S80), where regional grid utilisation weights are the average of regional shares of total export and import of energy according to Eq. (S81).

$$LCOEt_{total,r} = (LCOE_{sys,r} \cdot El_{consSys,r} + LCOE_{pros,r} \cdot El_{consPros,r}) / (El_{consSys,r} + El_{consPros,r}) \quad (S73)$$

$$LCOE_{sys,r} = LCOE_{prim,r} + LCOS_r + LCOC_r + LCOT_r + LCOFS_r \quad (S74)$$

$$LCOE_{pros,r} = LCOE_{prim,r} + LCOS_r - LCOFS_r \quad (S75)$$

$$LCOE_{gen,r} = \frac{\sum_{t=1}^{Gen} (CAPEX_t \cdot crf_t + OPEXfix_t) \cdot Cap_{t,r} + OPEXvar_t \cdot El_{gen,t,r}}{El_{gen,r}} \quad (S76)$$

$$LCOE_{prim,r} = \frac{LCOE_{gen,r} \cdot (El_{gen,r} - El_{curt,r} - El_{storLoss,r} - El_{transLoss,r})}{El_{cons,r}} \quad (S77)$$

$$LCOS_r = \left(\sum_{t=1}^{Stor} (CAPEX_t \cdot crf_t + OPEXfix_t) \cdot Cap_{t,r} + OPEXvar_t \cdot E_{out,t,r} + LCOE_{gen,r} \cdot El_{storLoss,r} \right) / El_{cons,r} \quad (S78)$$

$$LCOC_r = \frac{LCOE_{gen,r} \cdot El_{curt,r}}{El_{cons,r}} \quad (S79)$$

$$LCOT_r = RegShare_r \cdot \left(\sum_r^{Reg} \sum_{t=1}^{trans} (CAPEX_t \cdot crf_t + OPEXfix_t) \cdot Cap_{t,r} + OPEXvar_t \cdot El_{out,t,r} + LCOE_{gen,r} \cdot El_{transLoss,r} \right) / El_{cons,r} \quad (S80)$$

$$RegShare_r = 0.5 \cdot \frac{Import_r}{\sum_r Import_r} + 0.5 \cdot \frac{Export_r}{\sum_r Export_r} \quad (S81)$$

Abbreviations: region (*r*), total levelised cost of electricity in the system (*LCOEttotal*), centralised system levelised cost of electricity (*LCOEsys*), prosumer sector levelised cost of electricity (*LCOEpros*), centralised system electricity consumption (*ElconsSys*), prosumer sector electricity consumption (*ElconsPros*), consumed electricity LCOE (*LCOEprim*), levelised cost of stored electricity (*LCOS*), levelised cost of curtailed electricity (*LCOC*), levelised cost of

prosumer feed-in reimbursement ($LCOFS$), generated electricity LCOE ($LCOE_{gen}$), power generation technologies (Gen), storage technologies ($Stor$), power transmission technologies ($trans$), technology (t), capital expenditures ($CAPEX$), capital recovery factor for technology t (crf_t), annual fixed operational expenditures ($OPEX_{fix}$), variable operational expenditures ($OPEX_{var}$), installed capacity of the technology t (Cap_t), annual output for the technology t ($El_{gen,t}$), annual electricity generation (El_{gen}), annual electricity curtailment (El_{curt}), annual storage loss ($El_{storLoss}$), annual grid loss ($El_{transLoss}$), annual electricity consumption (El_{cons}), annual output of storage t ($E_{out,t}$), annual export of grid technology t ($El_{out,t}$), electricity exported by region r ($Export$), electricity imported by region r ($Import$), feed-in reimbursement ($feedInTarif$), electricity sold by prosumers to the grid ($EL_{prosToGrid}$).

The levelised cost of heat (LCOH) is calculated as the weighted average of the centralised and individual system LCOH according to Eq. (S82). The centralised heat system LCOH ($LCOH_{sys}$) and individual heat system LCOH ($LCOH_{ind}$) are calculated as the annualised cost of heat system equipment and annual cost of electricity consumption by heating equipment divided by total heat consumption according to Eqs. S79-S80. In both formulas, operational expenditures include the cost of electricity, fuel and GHG emissions per unit of generated heat. The heat systems also include parts of the fuel production facilities, which are used for fuel production for heat generators. Cogeneration plants costs are only included in the power system.

$$LCOH_{total,r} = (LCOH_{sys,r} \cdot He_{consSys,r} + LCOH_{ind,r} \cdot He_{consInd,r}) / (He_{consSys,r} + He_{consInd,r}) \quad (S82)$$

$$LCOH_{sys,r} = \left(\sum_{t=1}^{heat} (CAPEX_t \cdot crf_t + OPEX_{fix,t}) \cdot Cap_{t,r} + OPEX_{var,t} \cdot He_{out,t,r} + LCOE_{sys,r} \cdot El_{demSysHeat,r} \right) / He_{consSys,r} \quad (S83)$$

$$LCOH_{ind,r} = \left(\sum_{t=1}^{heat} (CAPEX_t \cdot crf_t + OPEX_{fix,t}) \cdot Cap_{t,r} + OPEX_{var,t} \cdot He_{out,t,r} + ElPrice_r \cdot El_{demIndHeat,r} \right) / He_{consInd,r} \quad (S84)$$

Abbreviations: region (r), total levelised cost of heat in the system ($LCOH_{total}$), centralised system levelised cost of heat ($LCOE_{sys}$), individual heat sector levelised cost of heat ($LCOH_{ind}$), centralised system heat consumption ($He_{consSys}$), individual heat sector heat consumption ($He_{consPros}$), heat generation technologies ($heat$), technology (t), capital expenditures ($CAPEX$), capital recovery factor for technology t (crf_t), annual fixed operational expenditures ($OPEX_{fix}$), variable operational expenditures ($OPEX_{var}$), installed capacity of the technology t (Cap_t), annual output for the technology t ($He_{out,t}$), centralised system levelised cost of electricity ($LCOE_{sys}$), retail price of electricity ($ElPrice$), electricity consumed by centralised heat system heaters ($El_{demSysHeat}$), electricity consumed by individual heat system heaters ($El_{demIndHeat}$).

For the integrated system, some capacities play a role in the power and heat supply systems, in this case these technologies costs are divided in between electricity and heat supply systems costs.

For levelised cost of electricity the annualised cost of the power supply are calculated considering electricity generation, storage, power transmission (in a multi nodal case) and PtX technologies (partially). The total power supply cost is then divided by total electricity

consumption by all sectors, including power-to-heat, power-to-fuel, power-to-mobility, industry and desalination demand, but excluding the electricity consumption by storage technologies. All CHP capacities costs are allocated to electricity cost as the heat is assumed to be a free by-product of the power production.

For levelised cost of heat, we calculate the annualised cost of the heat supply considering heat generation, storage and PtX (partially). The total heat production and storage cost is then divided by total heat consumption for heating, industrial processes, and e-fuels production.

The cost of fuel storage and PtX technologies, in particular for methane and hydrogen storage, electrolyzers, DAC, and methanation, are divided between electricity and heat cost accordingly to share respective fuels use for power and heat generation.

Weighted average cost of capital (WACC)

The WACC is varied between time and regions as shown in Figure S30 in a bottom-up procedure by defining a trend line for historic WACC values based on country-based lending rates [33] relative to the GDP per capita. Future WACC is estimated with the trendline approximation method as described by Keiner et al. [34]. The WACC for each country is calculated based on a relative return of investment of 100% of the lending rate and in a second case on an absolute return of investment of 6%. In both cases, a debt share of 70% is assumed. The chosen WACC is the higher value of both approaches. Country values are aggregated to major regions as average weighed by the total GDP.

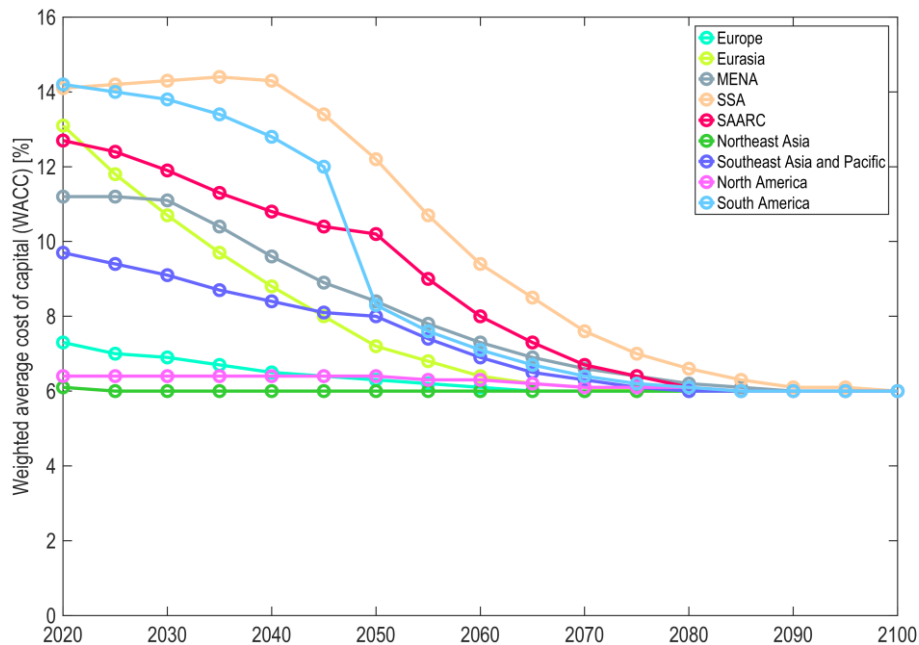


Figure S30. Assumptions for WACC varying by time step and region.

Supplementary note 3: Simplified method to estimate CDR demand, CDR demand scaling, and CDR allocation to major regions

Total CDR demand

The starting point for CDR demand estimation is the available CO₂ budget between 2020 and 2100, which has been estimated to ca. 300 GtCO₂ for a 1.5°C warming limit within the 83rd percentile in the Working Group I contribution to the AR6 [35]. First, insecurities of ca. 220 GtCO₂ are considered, leaving a net budget of ca. 80 GtCO₂. The residual fossil emissions of the energy-industry system is estimated to 680 GtCO₂ based on Keiner et al. [34], which is corrected by an expected 100 GtCO₂ of on-site CCS for mostly mineral CCS in the second half of the 21st century (cement). The net residual emissions are, therefore, estimated to 580 GtCO₂. Although not all emissions are expected to stay in the atmosphere, as ca. 44% of fossil emissions are currently taken up by oceans and land sinks [36].

For AFOLU emissions, CO₂ and N₂O as long-lived gases are considered in a cumulative fashion, while N₂O is converted to an CO₂-eq with a GWP100 factor of 273 [35]. In line with the expected overshoot pathway, the average values of the AR6 C2 scenarios are used as AFOLU emission pathways, leading to a total cumulative emission of 27 GtCO₂-eq.

The impact of aerosols is considered for black carbon (BC), organic carbon (OC), sulphate (SO₂), and ammonia (NH₃). The additional warming by eliminating fossil fuel-based aerosols is estimated to 0.5 K, based on a current cooling estimation of ca. 0.55 K, a reduction of BC emissions to 4% of today's value by 2050 based on air pollution estimations of a stringent defossilisation pathway [37], a reduction of organic carbon to 24% of today's value based on average C2 emission pathways of the AR6, an elimination of SO₂ emissions that comes with a deep defossilisation [37], and no change in NH₃ emissions as of today. The required change in atmospheric CO₂ concentration to offset the eliminated aerosol cooling is done by estimating the atmospheric CO₂ concentration in 2050 considering energy-industry and AFOLU CO₂ emissions, and using the logarithmic formula for radiative forcing and assuming an equilibrium climate sensitivity to estimate the required change in atmospheric CO₂, as described in Eq. (S85) and (S86) as described by Myhre et al. [38], Gregory and Forster [39], and Andrews et al. [40].

$$C = C_0 \cdot \exp\left(\frac{\Delta T}{\lambda \cdot 5.35}\right) \quad (\text{S85})$$

$$\lambda = \frac{ECS}{3.7 \text{ W} \cdot \text{m}^{-2}} \quad (\text{S86})$$

where C is the new atmospheric concentration, C_0 is the reference concentration, ΔT is the temperature difference, and ECS is the equilibrium climate sensitivity.

A climate sensitivity of 3.7 W·m⁻² is a standard value [41], and the ECS , although uncertain, is set to 3.0°C as a likely average value [35,42]. These assumptions lead to a required atmospheric CO₂ change of 48.6 ppm or 377 GtCO₂ at 7.77 GtCO₂/ppm (2.12 GtC per 1 ppm [42]).

The impact of short-lived methane (CH₄) is done by considering the remaining radiative forcing of CH₄ based on the emission trajectory by end of the century. The trajectory for 1.5°C is assumed to be in line with a 1.5°C target, so no additional radiative forcing of CH₄ has to be compensated. In the case of 1.0°C target, the remaining CH₄ forcing of 0.27 W/m² is considered

by a third. This simplified assumption is made based on the fact that the remaining forcing in line with a 1.5°C target versus a historical zero forcing of 0 W/m² has to be reduced by a 0.5°C equivalent, or a third of 1.5°C. The radiative forcing to be compensated is turned into an additional reduction of the atmospheric CO₂ concentration via Eq. (S85) and (S86).

The total gross CDR demand for 1.5°C is the sum of remaining budget, residual emissions, and aerosol compensation. However, when removing CO₂ from the atmosphere, and lowering atmospheric CO₂ concentrations, the ocean and land sink start to outgas CO₂ again, making removed CO₂ less effective. This has to be considered with a perturbation airborne fraction (PAF) [42,43], which increased the required CDR demand. The PAF is not linear or static and has to be calibrated based on the respective temperature anomaly. This validation was done using emission trajectories of LUT-DEMAND [34] for the same macro-economic scenario and the online MAGICC7 climate model (<https://live.magicc.org>) [44,45]. Finally, the calibration led to a PAF of 0.8 for the 1.5°C CDR demand and 0.75 for the 1.0°C CDR demand. The calibration results of MAGICC7 are shown in Figure S31 and Figure S32.

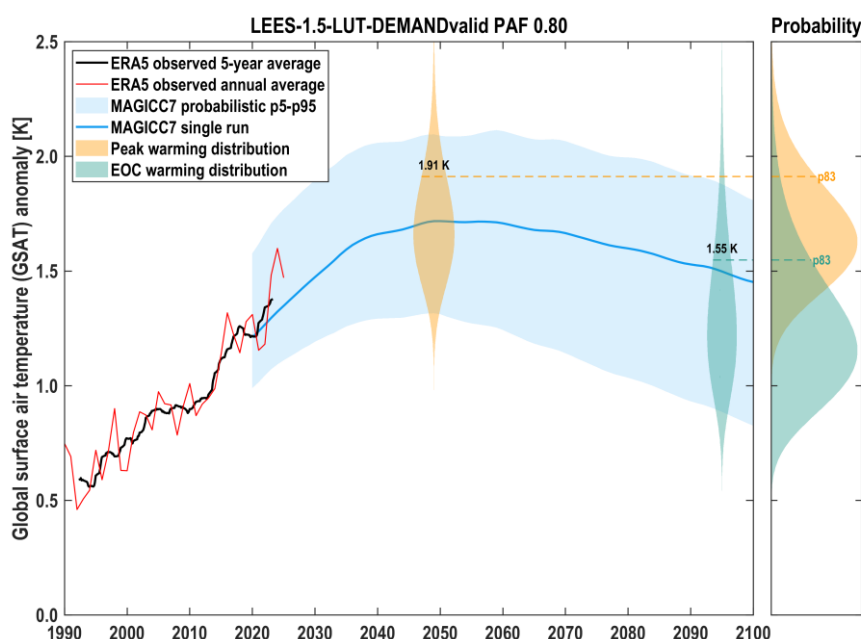


Figure S31. MAGICC7 calibration results for CDR demand estimation for the 1.5°C climate target.

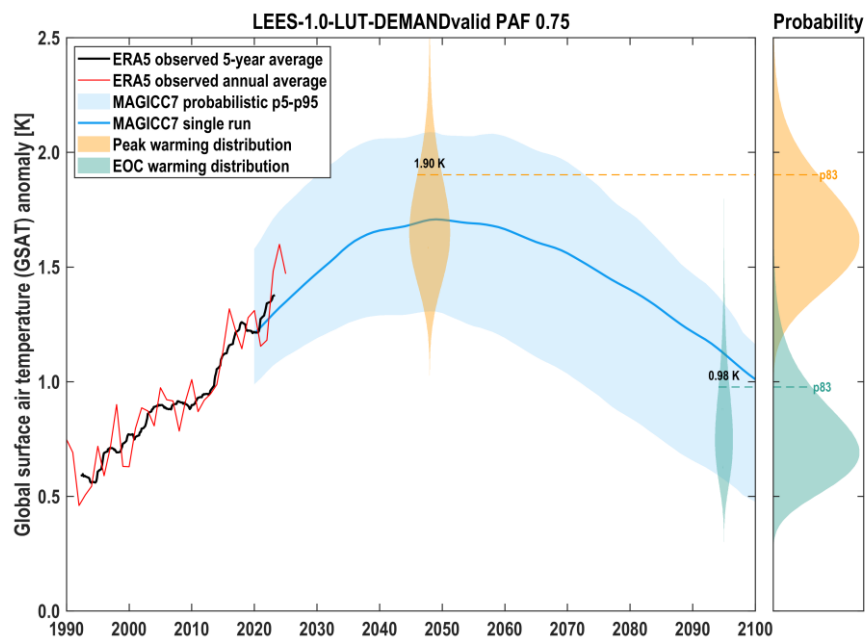


Figure S32. MAGICC7 calibration results for CDR demand estimation for the 1.5°C climate target.

The calibrated total CDR demand for 1.5°C was estimated with this simplified method to 724 GtCO₂, and for 1.0°C to 1682 GtCO₂.

CDR scaling

Scaling of CDR is assumed based on the premise that CDR should run as much on renewable electricity as possible, therefore, should not be scaled too early to avoid lock-in effects and give an incentive for further use of fossil fuels to be offset with CDR. However, it should also not be scaled too late to avoid too high growth rates and a realistic scaling of the CDR sector. Figure S33 shows the scaling of total annual global CDR demand.

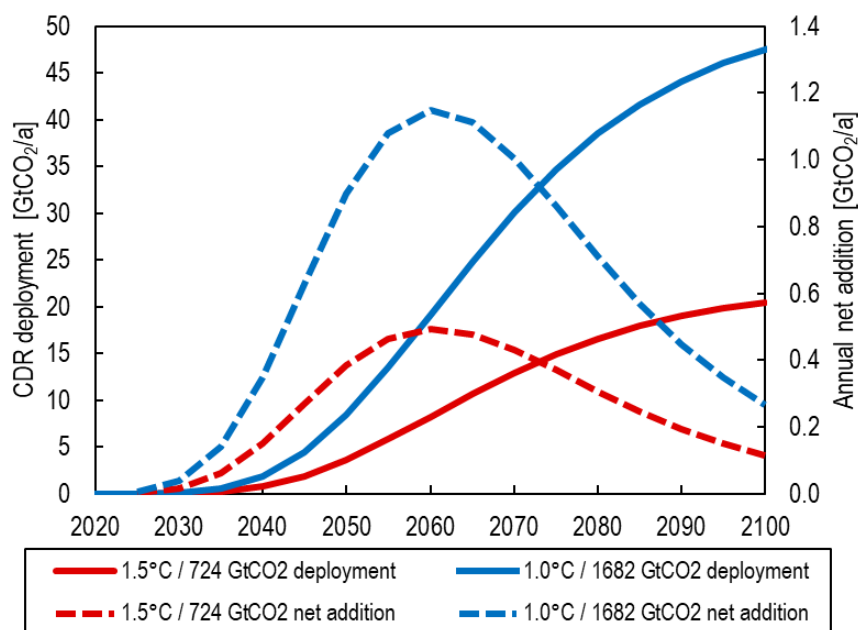


Figure S33. Scaling of annual CDR deployment by temperature target and year.

CDR allocation

Allocation of the CDR demand from a global demand to the 9 major regions is done by weighing different parameters representing societal preferences [46] including

- Total area availability
- Population
- Area per capita
- Historical emissions
- Current emissions
- Solar PV opportunity

Table S3 and Table S4 list the allocated CDR demand to major regions as used as input for CO₂SMOP. The actual CDR deployment may vary slightly due to model tolerances of CO₂SMOP.

Table S3. Allocated CDR demand to major regions for 1.5°C target. Values are rounded to two decimals in GtCO₂/a.

Region	2020	2025	2030	2035	2040	2045	2050	2055	2060	2065	2070	2075	2080	2085	2090	2095	2100
Europe	0.00	0.00	0.00	0.02	0.07	0.17	0.32	0.51	0.73	0.94	1.14	1.32	1.47	1.59	1.68	1.76	1.82
Eurasia	0.00	0.00	0.01	0.04	0.13	0.30	0.56	0.90	1.28	1.65	2.00	2.30	2.55	2.75	2.91	3.02	3.11
MENA	0.00	0.00	0.01	0.02	0.08	0.18	0.34	0.55	0.77	1.00	1.21	1.39	1.55	1.67	1.77	1.84	1.90
SSA	0.00	0.00	0.01	0.03	0.10	0.25	0.47	0.74	1.05	1.36	1.65	1.90	2.11	2.28	2.41	2.51	2.59
SAARC	0.00	0.00	0.00	0.02	0.05	0.11	0.22	0.35	0.49	0.64	0.78	0.90	0.99	1.08	1.14	1.19	1.23
NE-Asia	0.00	0.00	0.01	0.03	0.08	0.20	0.38	0.61	0.86	1.12	1.36	1.57	1.75	1.90	2.02	2.12	2.19
SE-Asia	0.00	0.00	0.00	0.02	0.08	0.18	0.34	0.55	0.77	1.00	1.22	1.40	1.56	1.69	1.79	1.87	1.93
N-America	0.00	0.00	0.01	0.04	0.13	0.31	0.59	0.94	1.34	1.73	2.10	2.41	2.68	2.90	3.07	3.20	3.30
S-America	0.00	0.00	0.01	0.03	0.09	0.22	0.41	0.66	0.94	1.23	1.49	1.72	1.91	2.08	2.21	2.31	2.39

Table S4. Allocated CDR demand to major regions for 1.0°C target. Values are rounded to two decimals in GtCO₂/a.

Region	2020	2025	2030	2035	2040	2045	2050	2055	2060	2065	2070	2075	2080	2085	2090	2095	2100
Europe	0.00	0.00	0.01	0.05	0.16	0.39	0.74	1.19	1.69	2.19	2.65	3.06	3.41	3.69	3.91	4.08	4.22
Eurasia	0.00	0.00	0.02	0.09	0.29	0.69	1.30	2.09	2.97	3.84	4.65	5.35	5.93	6.39	6.75	7.03	7.23
MENA	0.00	0.00	0.01	0.06	0.18	0.42	0.79	1.27	1.80	2.33	2.81	3.24	3.60	3.88	4.11	4.28	4.42
SSA	0.00	0.00	0.02	0.08	0.24	0.57	1.08	1.73	2.45	3.17	3.83	4.41	4.89	5.29	5.59	5.83	6.02
SAARC	0.00	0.00	0.01	0.04	0.11	0.27	0.51	0.81	1.15	1.49	1.80	2.08	2.31	2.50	2.65	2.76	2.85
NE-Asia	0.00	0.00	0.01	0.06	0.20	0.46	0.88	1.41	2.00	2.60	3.16	3.66	4.07	4.42	4.70	4.92	5.10
SE-Asia	0.00	0.00	0.01	0.06	0.18	0.42	0.79	1.27	1.80	2.33	2.83	3.26	3.63	3.92	4.16	4.35	4.49
N-America	0.00	0.00	0.02	0.10	0.30	0.72	1.36	2.19	3.10	4.02	4.87	5.61	6.23	6.73	7.13	7.43	7.66
S-America	0.00	0.00	0.01	0.07	0.21	0.51	0.96	1.54	2.19	2.85	3.46	3.99	4.45	4.82	5.12	5.36	5.55

Supplementary note 4: Description of the multi-objective CDR portfolio model

The following sequestration technologies are included in CO₂SMOP:

Abbreviation	Formula index	Description
GEO _{ON}	<i>GEO-ON</i>	Geological sequestration in sedimentary basins, onshore
GEO _{OFF}	<i>GEO-OFF</i>	Geological sequestration in sedimentary basins, offshore
MIN-IN _{ON}	<i>MIN-IN, ON</i>	In-situ mineralisation, onshore
MIN-IN _{OFF}	<i>MIN-IN, OFF</i>	In-situ mineralisation, offshore
MIN-EX	<i>MIN-EX</i>	Ex-situ mineralisation
SiC	<i>SiC</i>	Silicon carbide production
EW	<i>EW</i>	Enhanced weathering
BC	<i>BC</i>	Biochar
AF _{RF}	<i>AF-RF</i>	Rainfall-fed afforestation
AF _{DF}	<i>AF-DF</i>	Desalination-fed afforestation on arid land

Furthermore, the following technologies for carbon capture are included:

Abbreviation	Formula index	Description
DAC	<i>DAC</i>	Direct air capture CDR routes via DAC encompass the concept of direct air capture and sequestration (DACCS).
BioPSC	<i>BioPSC</i>	Bioenergy with carbon capture (point source capture) CDR routes via BioPSC encompass the concept of bioenergy with carbon capture and sequestration (BECCS).

CO₂ balance

To allow for the nonlinearity of afforestation, some flexibility for the total sequestration is needed, also since the CDR demand may not match the carbon sequestration curves of afforestation, which can lead to infeasibilities. Therefore, the main CDR balance is divided in two, according to Eq. (S87), (S88):

$$\forall y \in [2020, 2100]: \sum_{ts=1}^{nts} totS_{ts,y} - totS_{over,y} = totCDR_y \quad (S87)$$

$$\forall y \in [2020, 2100]: \sum_{ts=1}^{nts} totS_{ts,y} \leq totCDR_y \quad (S88)$$

$$\forall y \in [2020, 2100]: totS_{over,y} \leq \phi_{over} \cdot totCDR_y \quad (S89)$$

where

nts	Number of sequestration options
ts	Sequestration technology
y	Year / time step
$totS$	Total CO ₂ sequestration
$totS_{over}$	Total CO ₂ sequestration overshoot
$totCDR$	Total CDR demand
ϕ_{over}	Relative overshoot limitation (0-1)

Furthermore, the following balances described by Eq. (S90)-(S94) are included:

$$\forall y \in [2020, 2100]: totDAC_y + totBioPSC_y + totDirectS_y + totDirBioS_y - totS_{over,y} = totCDR_y \quad (S90)$$

$$\forall y \in [2020, 2100]: totS_{GEO-ON,y} + totS_{GEO-OFF,y} + totS_{MIN-IN,ON,y} + totS_{MIN-IN,OFF,y} + totS_{MIN-EX,y} + totS_{SiC,y} \leq totDAC_y \quad (S91)$$

$$\forall y \in [2020, 2100]: totS_{GEO-ON,y} + totS_{GEO-OFF,y} + totS_{MIN-IN,ON,y} + totS_{MIN-IN,OFF,y} + totS_{MIN-EX,y} + totS_{SiC,y} \leq totBioPSC_y \quad (S92)$$

$$\forall y \in [2020, 2100]: totS_{EW,y} = totDirectS_y \quad (S93)$$

$$\forall y \in [2020, 2100]: totS_{BC,y} + totS_{AF-DF} + totS_{AF-RF} = totDirBioS_y \quad (S94)$$

where

$totDAC$	Total sequestration with CO ₂ from DAC (DACCS)
$totBioPSC$	Total sequestration with CO ₂ from bioenergy + point source capture (BECCS)
$totDirectS$	Total direct sequestration (without primary or secondary capture process)
$totDirBioS$	Total direct biogenic sequestration (photosynthesis as the only process to capture CO ₂)

Eq. (S90) ensures that the total CDR demand is sufficiently covered, however, corrected by the overshoot. In combination with Eq. (S87) and (S88), the overshoot is limited to the afforestation options. Equation (S89) limits the overshoot relative to the total CDR demand.

Eq. (S91) defines the DACCS balance. Since all options can either be covered by DAC or bioenergy with point source capture, it is an inequality balance. The same logic is valid for the BECCS balance in Eq. (S92). Eq. (S93) defines direct sequestration, and Eq. (S94) defines direct sequestration in biomass. Direct sequestration is defined as the sequestration directly from the atmosphere, without a technological capture process between atmospheric CO₂ and the sequestration (see Keiner et al. [2] for the definition of primary and secondary capture processes).

Objective function

The objective of the linear model is to minimise the total score for the CDR portfolio for the predefined societal preference. Each sequestration option gets assigned a score between 0 and 1 for each time step based on lowest and highest values between the options. In the case of technology readiness and security, the values with the highest value (highest readiness or highest security) get the lowest score. For the objective value, a cohort sequestration cS of each technology is multiplied with the respective score. In this way, the average total installed

capacity including previously installed capacities are considered, so the procedure optimises not specific timesteps, but considers the legacy impact of an installation for future time steps. The total score sT for cost (C), energy (E), area (A), TRL (T), and security (S) is the sum of all technologies' scores, as can be seen in Eq. (S95)-(S99). The total scores are calculated for sequestration technologies ts and capture technologies tc (sequestration and capture technology: $ts \wedge tc$), except for security, as capture technologies are not relevant for permanence. The scores for capture technologies are calculated in the capture technology set but are re-normalised to express additional scores in the sequestration dimension.

$$sT_{ts \wedge tc}^C = \sum_{t=1}^{nts} \sum_{y=1}^{ny} cS_{t,y} \cdot s_{t,y}^C \quad (S95)$$

$$sT_{ts \wedge tc}^E = \sum_{t=1}^{nts} \sum_{y=1}^{ny} cS_{t,y} \cdot s_{t,y}^E \quad (S96)$$

$$sT_{ts \wedge tc}^A = \sum_{t=1}^{nts} \sum_{y=1}^{ny} cS_{t,y} \cdot s_{t,y}^A \quad (S97)$$

$$sT_{ts \wedge tc}^T = \sum_{t=1}^{nts} \sum_{y=1}^{ny} cS_{t,y} \cdot s_{t,y}^T \quad (S98)$$

$$sT_{ts}^S = \sum_{t=1}^{nts} \sum_{y=1}^{ny} cS_{t,y} \cdot s_{t,y}^S \quad (S99)$$

The final objective value/score $sObj$ is calculated as described in Eq. (S100):

$$sObj = \gamma_{sp,ts \wedge tc}^C \cdot sT_{ts \wedge tc}^C + \gamma_{sp,ts \wedge tc}^E \cdot sT_{ts \wedge tc}^E + \gamma_{sp,ts \wedge tc}^A \cdot sT_{ts \wedge tc}^A + \gamma_{sp,ts \wedge tc}^T \cdot sT_{ts \wedge tc}^T + \gamma_{sp,ts}^S \cdot sT_{ts}^S \quad (S100)$$

where

- γ_{sp}^C Societal preference weight for cost
- γ_{sp}^E Societal preference weight for energy
- γ_{sp}^A Societal preference weight for area
- γ_{sp}^T Societal preference weight for TRL
- γ_{sp}^S Societal preference weight for security (permanence)

Supplementary note 5: CDR technology potentials

The following parts describe how the global potential for different CDR options have been obtained and visualise the potentials in a gridded map. For CDR options with a cumulative potential, and extraction rate of 1%/a is assumed as a conservative assumption based on current typical 2%/a extraction rates of the oil and gas industry [47]. Onshore potentials are estimated for all nodes included in the major region's land area (see Figure S1) and offshore potentials are estimated within each region's exclusive economic zone (EEZ) (see Figure S2).

The availability of CDR sequestration options is limited by several factors:

- Protected areas [48] are excluded.
- Areas with a sea depth of more than 3000 m are excluded. This is based on current maximum drilling depths of modern oil and gas rigs [49,50].
- Areas with a population density of more than 250 persons/km² [51] are excluded to avoid overestimation of the available area in densely populated areas.
- The entire Antarctic is excluded based on the Madrid protocol of 1991 (The Protocol on Environmental Protection to the Antarctic Treaty) [52].

Figure S34 shows a map of the available nodes in $0.45^\circ \times 0.45^\circ$ resolution with the available nodes based on the filtering explained above. This filter is applied to theoretically available nodes as presented in the following for each sequestration option.

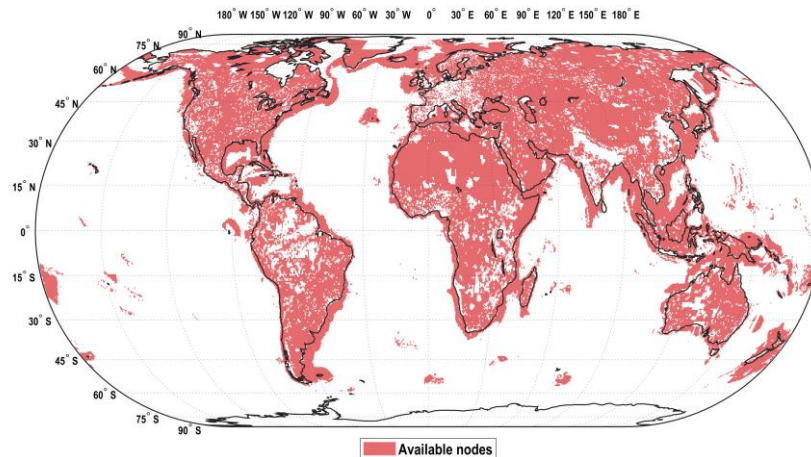


Figure S34. Available nodes for CDR deployment applied as filter for limiting the theoretical potential to socio-technological potential.

Geological sequestration

Figure S35 shows the theoretical potential for geological sequestration, which has been derived as following:

- Global geological CO₂ storage availability map by combining sedimentary basin data from Bradshaw and Dance [53] and IPCC [54] with the world total petroleum system geological shapefile [55].
- Area of each of the global $0.45^\circ \times 0.45^\circ$ grid cell (400 × 800 nodes resolution).
- Interpolated sedimentary thickness data from Laske and Masters [56] to match the model grid resolution.

- Nodal potential by applying a storage capacity factor of $0.037 \text{ GtCO}_2/\text{km}^3$ ([57], lower estimation) to the calculated sedimentary volumes.

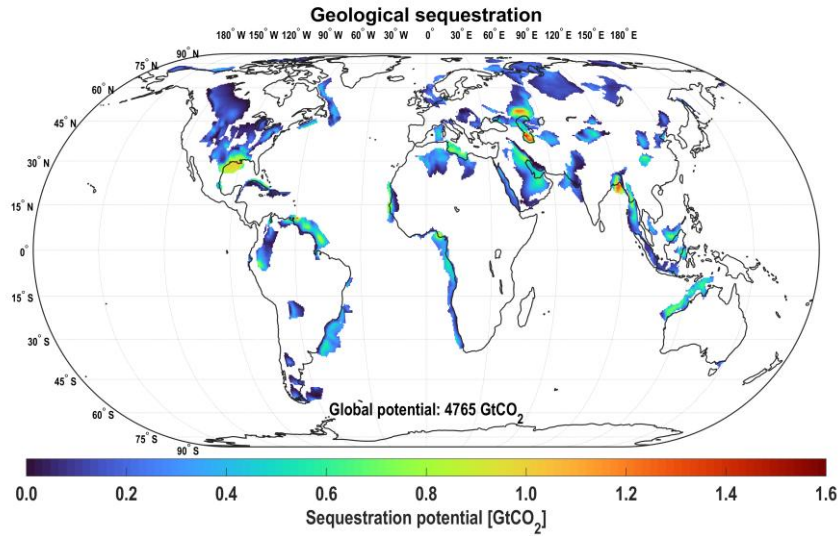


Figure S35. Theoretical potential for geological sequestration in $0.45^\circ \times 0.45^\circ$ resolution.

In-situ mineralisation

Figure S36 shows the theoretical potential of in-situ mineralisation which has been derived as following:

- Global mineralisation availability map by converting the large igneous provinces dataset by Johanson et al. [58] to the $0.45^\circ \times 0.45^\circ$ (400×800) model grid.
- Volume of each suitable grid cell using the grid-cell area and an assumed average basalt layer thickness of 500 m [59].
- Nodal CO₂ mineralisation potential by applying a conservative sequestration capacity of $10 \text{ kgCO}_2/\text{m}^3$ for basalt [59].

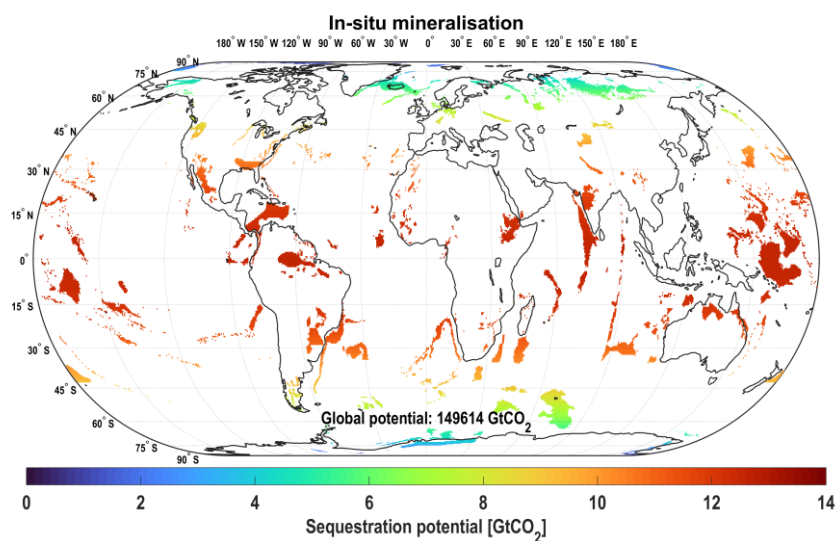


Figure S36. Theoretical potential for in-situ mineralisation in $0.45^\circ \times 0.45^\circ$ resolution.

Ex-situ mineralisation

The potential for ex-situ mineralisation is based on industrial waste per major region and taken from Mühlbauer et al. [60]. No gridded data are available.

Electricity-based silicon carbide

e-SiC would require detailed industry potentials and market outlooks to determine the future potential for an SiC market [60]. Theoretically, the global potential could be as high as $13.7 \text{ GtCO}_2 \text{ a}^{-1}$ if e-SiC is used as a substitution for construction sand [61]. For this study, no potential for e-SiC is assumed. This option is, however, implemented in LUT-ESTM for future use.

Enhanced weathering

Figure S37 shows the theoretical potential of enhanced weathering (EW) which has been derived as following:

- Enhanced weathering suitability map by converting Copernicus land-cover data [62] to the $0.45^\circ \times 0.45^\circ$ (400×800) model grid and selecting cropland.
- Area of each grid cell.
- Temperature-dependent weathering factor following Streffer et al. [63].
- Estimated the annual CO_2 sequestration potential by combining the temperature correction with the area demand of $850 \text{ km}^2/(\text{MtCO}_2 \text{ a}^{-1})$ reported by Keiner et al. [64].

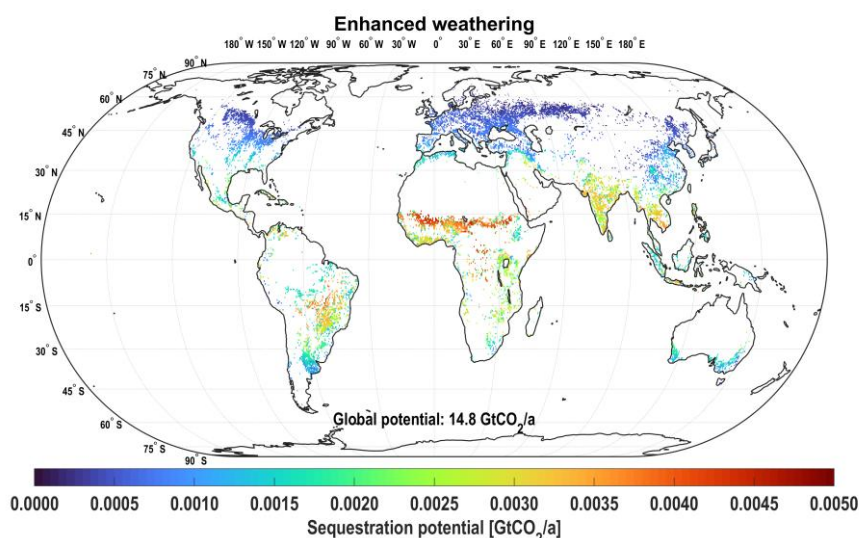


Figure S37. Theoretical potential for enhanced weathering in $0.45^\circ \times 0.45^\circ$ resolution.

Biochar

Figure S38 shows the theoretical potential for biochar (BC) which has been derived as following:

- Biochar suitability map from Copernicus land-cover data [62], considering cropland classes excluding bare land.
- Area of each $0.45^\circ \times 0.45^\circ$ grid cell.
- Annual CO_2 sequestration potential using an area demand of $580 \text{ km}^2 (\text{MtCO}_2 \text{ a}^{-1})$ [64].

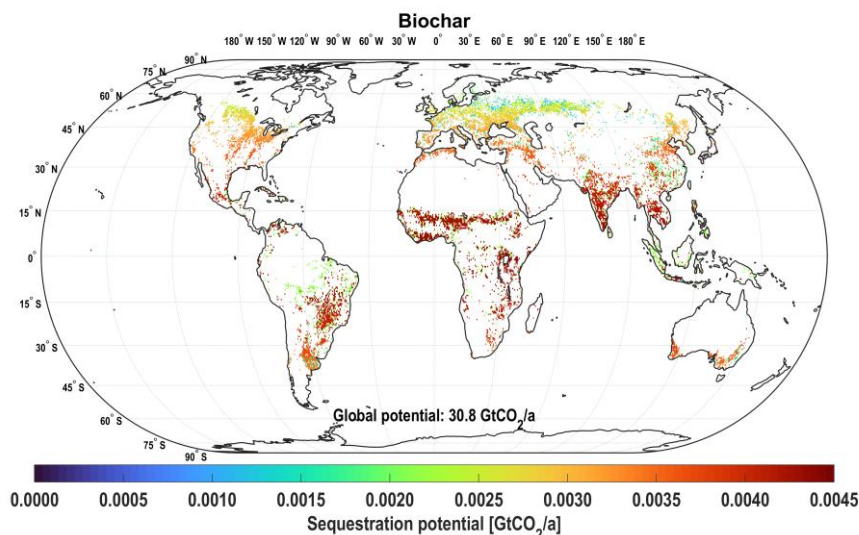


Figure S38. Theoretical potential for biochar sequestration in $0.45^\circ \times 0.45^\circ$ resolution.

Rainfed afforestation

Figure S39 shows the theoretical potential of rainfed afforestation (AF_{RF}) which has been derived as following:

- Afforestation suitability map by converting global forest loss driver data by Sims et al. [65] to the $0.45^\circ \times 0.45^\circ$ (400×800) model grid.
- Only non-temporary forest loss drivers are considered (hard commodities and shifting cultivation) while excluding temporary or regenerating forest loss (e.g., wildfire, forestry, logging, settlements, permanent agriculture).
- Available reforestation area in each grid cell from the fraction of eligible forest loss drivers and the grid-cell area.
- Annual CO₂ sequestration potential using an area demand of $800 \text{ km}^2 \text{ (MtCO}_2 \text{ a)}^{-1}$ [64].

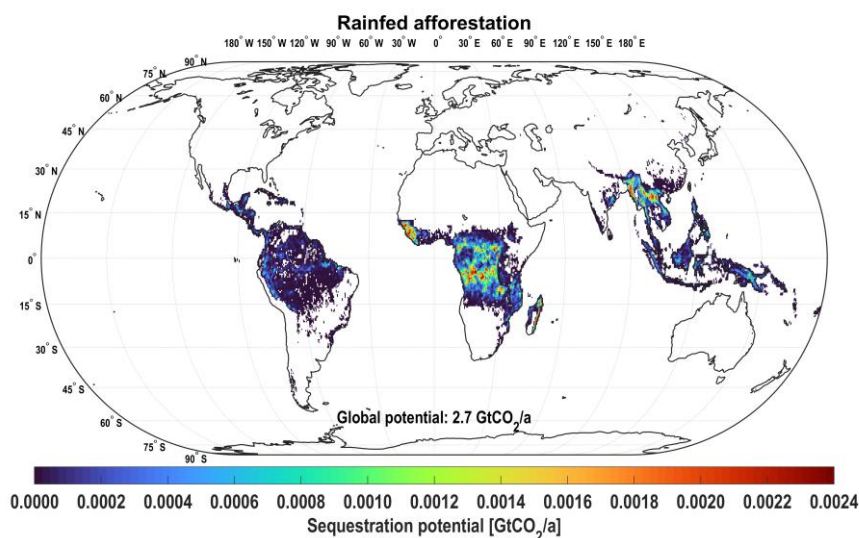


Figure S39. Theoretical potential for rainfed afforestation in $0.45^\circ \times 0.45^\circ$ resolution.

Desalination-fed afforestation

Figure S40 shows the theoretical potential for desalination-fed afforestation (AF_{DF}) which has been derived as following:

- Arid forestation with desalinated freshwater suitability map by Caldera and Breyer [66].
- Area of each $0.45^\circ \times 0.45^\circ$ grid cell.
- Annual CO_2 sequestration potential using an area demand of $350 \text{ km}^2 (\text{MtCO}_2 \text{ a})^{-1}$ and assuming 20% potential canopy cover [64,66].

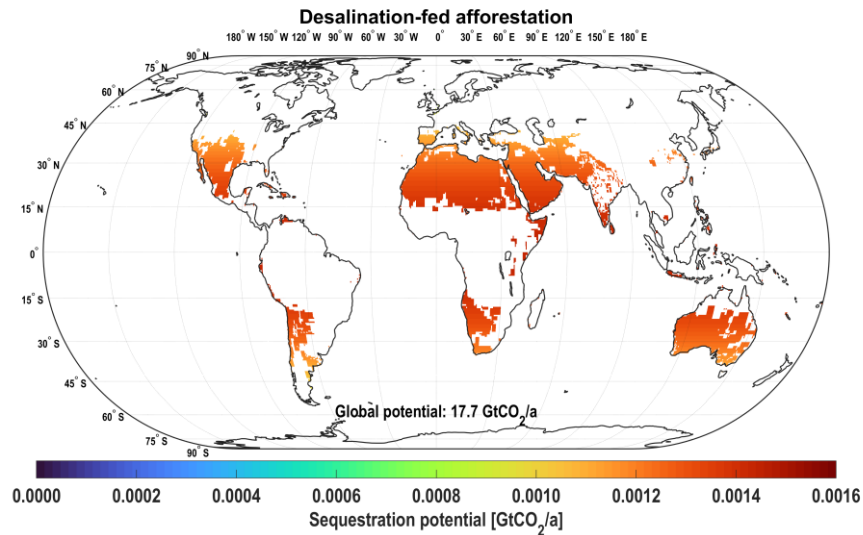


Figure S40. Theoretical potential for desalination-fed afforestation in $0.45^\circ \times 0.45^\circ$ resolution.

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