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Supplement of

MESSAGEix-Materials v1.1.0: representation of material flows and stocks in an integrated assessment model

Gamze Ünlü et al.

Correspondence to: Gamze Ünlü (unlu@iiasa.ac.at)

S1 Data Sources in MESSAGEix-Materials for Parametrization

Below table summarizes the data sources and their purpose of use for different industry sectors that are represented in MESSAGEix-Materials.

Table S1 Techno-economic data sources for the industries in MESSAGEix-Materials

Industry	**Source**	**Description**
Aluminium	IEA Energy Technology Transitions for Industry, 2009 (https://www.iea.org/reports/energy-technology-transitions-for-industry)	Choice of relevant industry technologies
	IEA ETSAP Technology Brief I10, 2012 (https://iea-etsap.org/E-TechDS/PDF/I10_AlProduction_ER_March2012_Final%20GSOK.pdf)	Techno-economic parameters, emission factors
	JRC Report Energy Efficiency and GHG Emissions: Prospective Scenarios for the Aluminium Industry (https://publications.jrc.ec.europa.eu/repository/handle/JRC96680)	Techno-economic parameters
	International Aluminum Institute (https://alucycle.world-aluminium.org/public-access/)	Material flows into product level, available end-of-life materials, trade calibration
	Idoine, N.E., Raycraft, E.R., Price, F., Hobbs, S.F., Deady, E.A., Everett, P., Shaw, R.A., Evans, E.J., and Mills, A.J.: World mineral production 2017-21, British Geological Survey, Nottingham, UK, 98pp., ISBN 9780852727973, 2023.	Historical data
	World Bank International Trade Costs (https://databank.worldbank.org/source/escap-world-bank-international-trade-costs) The United Nations Conference for Trade and Development (UNCTAD) https://unctadstat.unctad.org/datacentre/reportInfo/US.TransportCosts https://unctadstat.unctad.org/datacentre/dataviewer/US.TransportCosts	Trade costs
Chemicals	IKARUS Model https://www.energyplan.eu/othertools/national/ikarus/	Refinery techno-economic parameters
	PRELIM Model https://www.ucalgary.ca/energy-technology-assessment/open-source-models/prelim	Refinery techno-economic parameters
	IEA The Future of Petrochemicals, 2018 (https://www.iea.org/reports/the-future-of-petrochemicals)	Determining relevant industry technologies
	IEA Energy Technology Perspectives 2020 (https://www.iea.org/reports/energy-technology-perspectives-2020)	Determining relevant industry technologies, techno-economic parameters
	IEA Energy Technology Transitions for Industry, 2009 (https://www.iea.org/reports/energy-technology-transitions-for-industry)	Determining relevant industry technologies

	IEA ETSAP Bioethylene Production (https://iea-etsap.org/E-TechDS/PDF/I13IR_Bioethy_MB_Jan2013_final_GSOK.pdf)	Techno-economic parameters
	IEA ETSAP Oil Refineries (https://iea-etsap.org/E-TechDS/PDF/P04_Oil%20Ref_KV_Apr2014_GSOK.pdf)	Techno-economic parameters
	Tuna, P., Hulteberg, C., and Ahlgren, S.: Techno-economic assessment of nonfossil ammonia production, Environ. Prog. Sustain., 33, 1290–1297, https://doi.org/10.1002/EP.11886, 2014.	Techno-economic parameters
	IEA Ammonia Technology Roadmap, 2021 (https://www.iea.org/reports/ammonia-technology-roadmap)	Historical data
	Yara Fertilizer Industry Handbook, 2018 https://www.yara.com/siteassets/investors/057-reports-and-presentations/other/2018/fertilizer-industry-handbook-2018.pdf/	Historical data
	FAOSTAT fertilizer trade, 2018 https://www.fao.org/in-focus/remaining-fertilizer-trade-tracker/en IEA Energy Technology Transitions for Industry, 2009 (https://www.iea.org/reports/energy-technology-transitions-for-industry)	Historical trade data Conventional technologies techno-economic parameters
	Carina Oliveira. (2021). ADVANCED METHANOL TO OLEFINS PROCESS - TECHNOLOGY FACTSHEET. TNO. https://energy.nl/media/data/Technology-Factsheet-Advanced-methanol-to-olefins.pdf	Techno-economic parameters
	Dimian, A. C., & Bildea, C. S. (2018). Energy efficient methanol-to-olefins process. Chemical Engineering Research and Design, 131, 41–54. https://doi.org/10.1016/J.CHERD.2017.11.009	Techno-economic parameters
	Guillaume Gaulier & Soledad Zignago, 2010. "BACI: International Trade Database at the Product-Level. The 1994-2007 Version," CEPII Working Paper 2010- 23, October 2010, CEPII.	Historical trade data
	Geyer, R., Jambeck, J. R., & Law, K. L. (2017). Production, use, and fate of all plastics ever made. Science Advances, 3(7). https://doi.org/10.1126/SCIADV.1700782/SUPPL_FILE/1700782_SM.PDF	Techno-economic parameters
	Levi, P. G., & Cullen, J. M. (2018). Mapping Global Flows of Chemicals: From Fossil Fuel Feedstocks to Chemical Products. Environmental Science and Technology, 52(4), 1725–1734. https://doi.org/10.1021/acs.est.7b04573	Material flow data
	METI (2016), Future Supply and Demand Trend of Petrochemical Products Worldwide, Tokyo, www.meti.go.jp/policy/mono_info_service/mono/chemistry/sekkajyukyuudoukou201506.html	Historical data
	INTRATEC, https://www.intratec.us/products/plant-location-factors	Regional differentiation of costs
	Methanol Institute: Global Methanol Supply and Demand Balance: https://www.methanol.org/methanol-price-supply-demand/, last_access: 2023, 2022.	Historical data
	Poluzzi, A., Guandalini, G., Guffanti, S., Martinelli, M., Moioli, S., Huttenhuis, P., Rexwinkel, G., Palonen, J., Martelli, E., Groppi, G., & Romano, M. C. (2022). Flexible Power and Biomass-To-Methanol Plants With Different Gasification Technologies. Frontiers in Energy Research, 9, 978. https://doi.org/10.3389/FENRG.2021.795673/BIBTEX	Techno-economic parameters

	Renewable Energy Agency (IRENA), I., & Methanol Institute. (2021). INNOVATION OUTLOOK RENEWABLE METHANOL. www.irena.org	Techno-economic parameters
	Schemme, S., Breuer, J. L., Köller, M., Meschede, S., Walman, F., Samsun, R. C., Peters, R., & Stolten, D. (n.d.-a). H 2-based synthetic fuels: A techno-economic comparison of alcohol, ether and hydrocarbon production. https://doi.org/10.1016/j.ijhydene.2019.05.028	Techno-economic parameters
	S&P Global. (2020). Chemical Economics Handbook – Methanol. https://www.spglobal.com/commodityinsights/en/ci/products/methanol-chemical-economics-handbook.html	Historical data
Power Sector	Arvesen, A., Luderer, G., Pehl, M., Bodirsky, B. L., and Hertwich, E. G.: Deriving life cycle assessment coefficients for application in Integrated Assessment Modelling, Environ. Modell. Softw., 99, 111–125, https://doi.org/10.1016/j.envsoft.2017.09.010, 2018.	Material intensities
	Kalt, G., Thunshirn, P., Wiedenhofer, D., Krausmann, F., Haas, W., and Haberl, H.: Material stocks in global electricity infrastructures – An empirical analysis of the power sector's stock-flow-service nexus, Resources, Conservation and Recycling, 173, 105723, DOI: 10.1016/j.resconrec.2021.105723, 2021.	Hydro-power material intensity
Iron and steel	OECD steelmaking capacity database https://stats.oecd.org/Index.aspx?datasetcode=STI_STEEL_MAKINGCAPACITY World Steel Association (https://www.worldsteel.org/en/dam/jcr:0474d208-9108-4927-ace8-4ac5445c5df8/World+Steel+in+Figures+2017.pdf)	Historical data, Past capacity and production, trade calibration
	https://www.hellenicshippingnews.com/wp-content/uploads/2017/11/Market-dry-bulk-freight-rates.jpg World Bank, International Trade Costs (https://databank.worldbank.org/source/escap-world-bank-international-trade-costs) The United Nations Conference for Trade and Development (UNCTAD) https://unctadstat.unctad.org/datacentre/reportInfo/US.TransportCosts https://unctadstat.unctad.org/datacentre/dataviewer/US.TransportCosts	Trade costs
	IEA ETSAP Technology Brief I02, 2010 (https://iea-etsap.org/E-TechDS/PDF/I02-Iron&Steel-GS-AD-gct.pdf)	Techno-economic parameters
	IEA Energy Technology Transitions for Industry, 2009 (https://www.iea.org/reports/energy-technology-transitions-for-industry)	Techno-economic parameters
	Otto et al., 2017; Perpiñán et al., 2023 ; Fan & Friedmann, 2021; Gielen, 2003; Keys et al., 2019, IEA Iron and Steel Technology Roadmap	CCS parameters
	Wang et al., 2021; Devlin et al., 2023; Toktarova et al., 2022; Pimm et al., 2021; Lopez et al., 2022	Hydrogen steel making parametrization
Cement	Cement Statistics and Information (USGS) (https://pubs.usgs.gov/periodicals/mcs2020/mcs2020-cement.pdf)	Historical data, regional production
	2019 Activity Report (Cembureau) (http://www.cembureau.eu/media/clkdda45/activity-report-2019.pdf)	Historical data
	ADVANCE Modeling Guide for the Cement Industry, 2016 (http://fp7-advance.eu/content/industrial-sector-cement-guideline)	Techno-economic parameters, costs for CCS, emission factors

	Voldsund, M., Gardarsdottir, S., De Lena, E., Pérez-Calvo, J.-F., Jamali, A., Berstad, D., Fu, C., Romano, M., Roussanaly, S., Anantharaman, R., Hoppe, H., Sutter, D., Mazzotti, M., Gazzani, M., Cinti, G., and Jordal, K.: Comparison of Technologies for CO2 Capture from Cement Production—Part 1: Technical Evaluation, Energies, 12, 559, https://doi.org/10.3390/en12030559, 2019. Gardarsdottir, S., De Lena, E., Romano, M., Roussanaly, S., Voldsund, M., Pérez-Calvo, J.-F., Berstad, D., Fu, C., Anantharaman, R., Sutter, D., Gazzani, M., Mazzotti, M., and Cinti, G.: Comparison of Technologies for CO2 Capture from Cement Production—Part 2: Cost Analysis, Energies, 12, 542, https://doi.org/10.3390/en12030542, 2019.	Techno-economic parameters of CCS technologies
	Methodology for the free allocation of emission allowances in the EU ETS post 2012, 2009 (https://climate.ec.europa.eu/system/files/2016-11/bm_study-project_approach_and_general_issues_en.pdf) IEA ETSAP - Technology Brief I03, 2010 (https://iea-etsap.org/E-TechDS/PDF/I03_cement_June_2010_GS-gct.pdf)	Historical data, emission factors

S2 Regions in MESSAGEix-Materials

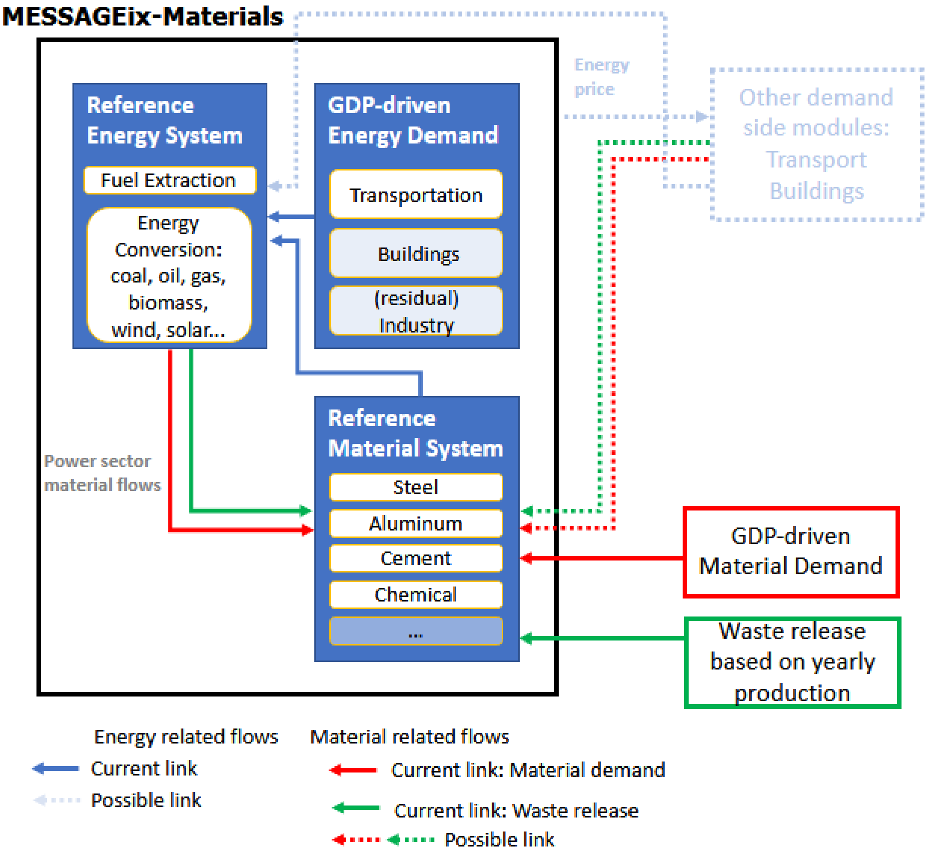
Table S2 Regions in MESSAGEix-Materials

NAM	North America	Canada, Guam, Puerto Rico, United States of America, Virgin Islands
WEU	Western Europe	Andorra, Austria, Azores, Belgium, Canary Islands, Channel Islands, Cyprus, Denmark, Faeroe Islands, Finland, France, Germany, Gibraltar, Greece, Greenland, Iceland, Ireland, Isle of Man, Italy, Liechtenstein, Luxembourg, Madeira, Malta, Monaco, Netherlands, Norway, Portugal, Spain, Sweden, Switzerland, Turkey, United Kingdom
PAO	Pacific OECD	Australia, Japan, New Zealand
EEU	Central and Eastern Europe	Albania, Bosnia and Herzegovina, Bulgaria, Croatia, Czech Republic, The former Yugoslav Rep. of Macedonia, Hungary, Poland, Romania, Slovak Republic, Slovenia, Yugoslavia, Estonia, Latvia, Lithuania
FSU	Former Soviet Union	Armenia, Azerbaijan, Belarus, Georgia, Kazakhstan, Kyrgyzstan, Republic of Moldova, Russian Federation, Tajikistan, Turkmenistan, Ukraine, Uzbekistan
RCPA	Centrally Planned Asia	Cambodia, , Korea (DPR), Laos (PDR), Mongolia, Viet Nam
CHN	China	China (incl. Hong Kong)
SAS	South Asia	Afghanistan, Bangladesh, Bhutan, India, Maldives, Nepal, Pakistan, Sri Lanka
PAS	Other Pacific Asia	American Samoa, Brunei Darussalam, Fiji, French Polynesia, Gilbert-Kiribati, Indonesia, Malaysia, Myanmar, New Caledonia, Papua, New Guinea, Philippines, Republic of Korea, Singapore, Solomon Islands, Taiwan (China), Thailand, Tonga, Vanuatu, Western Samoa
MEA	Middle East and North Africa	Algeria, Bahrain, Egypt (Arab Republic), Iraq, Iran (Islamic Republic), Israel, Jordan, Kuwait, Lebanon, Libya/SPLAJ, Morocco, Oman, Qatar, Saudi Arabia, Sudan, Syria (Arab Republic), Tunisia, United Arab Emirates, Yemen
LAM	Latin America and the Caribbean	Antigua and Barbuda, Argentina, Bahamas, Barbados, Belize, Bermuda, Bolivia, Brazil, Chile, Colombia, Costa Rica, Cuba, Dominica, Dominican Republic, Ecuador, El Salvador, French Guyana, Grenada, Guadeloupe, Guatemala, Guyana, Haiti, Honduras, Jamaica, Martinique, Mexico, Netherlands Antilles, Nicaragua, Panama, Paraguay, Peru, Saint Kitts and Nevis, Santa Lucia, Saint Vincent and the Grenadines, Suriname, Trinidad and Tobago, Uruguay, Venezuela
AFR	Sub-Saharan Africa	Angola, Benin, Botswana, British Indian Ocean Territory, Burkina Faso, Burundi, Cameroon, Cape Verde, Central African Republic, Chad, Comoros, Cote d'Ivoire, Congo, Democratic Republic of Congo, Djibouti, Equatorial Guinea, Eritrea, Ethiopia, Gabon, Gambia, Ghana, Guinea, Guinea-Bissau, Kenya, Lesotho, Liberia, Madagascar, Malawi, Mali, Mauritania, Mauritius, Mozambique, Namibia, Niger, Nigeria, Reunion, Rwanda, Sao Tome and Principe, Senegal, Seychelles, Sierra Leone, Somalia, South Africa, Saint Helena, Swaziland, Tanzania, Togo, Uganda, Zambia, Zimbabwe |

S3 Integration of MESSGAEix-Materials

Figure S1 shows the integration of MESSAGEix-Materials which is depicted as Reference Material System with a MESSAGEix-GLOBIOM base scenario which is referred as Reference Energy System. GDP-driven energy demand consists of transportation, buildings and the residual industry for the sectors that are not explicitly represented in the model. Material demand is either GDP driven and exogenously provided or can be endogenously represented such as the power sector that is connected to the Reference Material System (see section 2.4). Similarly, other demand side modules such as transport and buildings can be also added to the framework and provide information on material demand and end-of-life material release which is not available in this version.

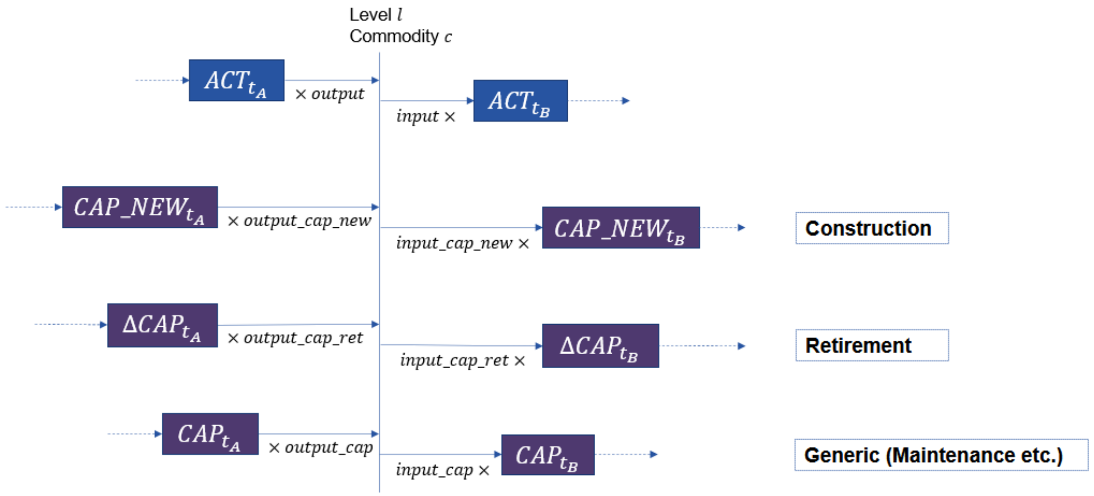
Figure S1 Integration of MESSAGEix-Materials in MESSAGEix framework



S4 Extension of MESSAGEix Model Formulation

It is mentioned in the main text that the MESSAGEix formulation currently can represent flows related to the activity (operation) of the technologies such as the energy flows. Figure S2 shows the newly added parameters to the model formulation and how they work to represent material flows related to the technology capacity. Boxes represent the decision variables in the model. Blue boxes that represent activity (ACT) and the purple ones that represent capacity (CAP) are already part of the current model formulation together with the parameters *input* and *output* associated with technology activity (e.g., coal input to produce 1 GWh of electricity). The parameters associated with the capacity are newly added. These flows can be either related to newly built capacity (CAP_NEW) or existing cumulative capacity (CAP). Material flows related to construction use CAP_NEW variable while material flows related to retirement and maintenance use CAP variable in the formulation.

Figure S2 Change of model formulation to represent the material flows related to technology capacity



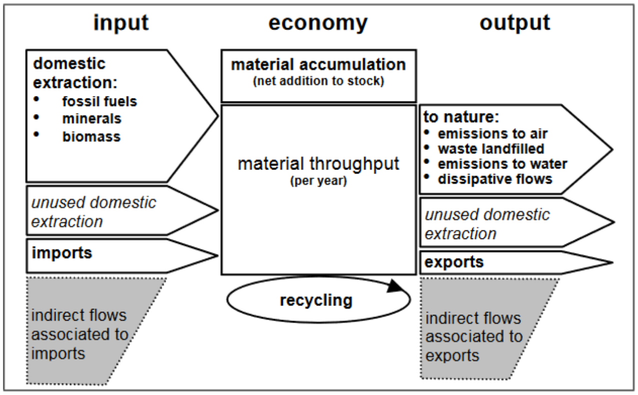
ACT: Activity of a technology (yearly average over period duration)
CAP_NEW: Newly installed capacity (yearly average over period duration)
CAP: Total maintained capacity in an operational and vintage year combination
input: Relative share of input per unit of activity
output: Relative share of output per unit of activity
output_cap_new: Relative share of output per unit of new capacity built. (Material released during the construction of a technology).
input_cap_new: Relative share of input per unit of new capacity built. (Material needed to build a certain capacity of a technology).
output_cap_ret: Relative share of output per unit of capacity retired. (Scrap material that becomes available as a result of the retirement of a technology.)
input_cap_ret: Relative share of input per unit of capacity retired. (Material needed for the retirement of certain capacity of a technology.)
output_cap: Relative share of output per unit of capacity. (Material released during the operation of a technology.)
input_cap: Relative share of input per unit of capacity. (Material needed during the lifetime of a technology for example for maintenance.)

S5 General Material Cycle System Definition in Economy-wide Material Flow Analysis

The system boundary in economy-wide material flow accounting is defined along the System of National Accounts as seen in Fig. S3, starting from: 1. the extraction of primary (i.e., raw, crude or virgin) materials from the national environment and the discharge of materials to the national environment; 2. the political (administrative) borders that determine material flows to and from the rest of the world (imports and exports). Natural flows into and out of a geographical territory are excluded. The key unit of measurement in MFA are metric tons (Krausmann, 2017; Graedel, 2019). Economy-wide material flow accounts (EW-MFA) are rich empirical databases reporting domestic extraction and physical trade for all economies of the world, differentiating 50-60 raw material types (Eurostat, 2018; UNEP and IRP, 2023). From this data, policy-relevant headline indicators are being derived, such as “Domestic Material Consumption” (DMC), in combination with an MRIO, the “material footprint” (MF), as well as relative indicators such as “Resource Productivity” (GDP/DMC or GDP/MF). These indicators are widely used for European and international policy such as in European Green Deal or SDG targets 8 and 12 (Lenzen et al.,2022; European Commission, 2020). Recently, EW-MFA has been further developed by integrating different socio-economic uses of material flows, material stock dynamics, as well as waste and GHG emissions, which enables analysing circular economies (Haas et al., 2020; Kovanda, 2021; Schandl and Miatto, 2018), as well as deriving policy-relevant circular economy indicators for national economies (Mayer, 2019; European Commission, 2023; BMK, 2022).

Recently, research has begun expanding this framework towards explicitly including material stocks and industrial processes and supply chains, opening up the black of “the economy” shown below. This required merging principles of material flow analysis which is relatively flexible, with the standardized economy-wide approach; resulting in a novel approach termed economy-wide material and energy flow analysis (Plank, 2022; Wiedenhofer 2019). For the MESSAGEix-Materials module, we draw on these recent developments to develop the integrative system definition shown in Fig. 2 in the main text.

Figure S3 Economy-wide material balance scheme (excluding air and water flows) (European Commission, 2001)



S6 Additional Details for Integrative System Definition

Table S3 provides additional information on the Fig. 2 that is presented in the main text. For each process, the mass balance is shown based on the inflows and outflows in the column "Mass Balance". In addition, some generic flows that require more explanation about these processes are also listed in the column "Additional Description of Flows". For example, the term waste is used in general for many processes and the details about the type of waste are provided. The column "Material Levels for Outflows in the Model" shows to which "level" the outflows from the processes go in the model. The definition of model levels and the Reference Material System approach is explained in Sect. 2.3.

Table S3 Additional Details for Processes in Integrative System Definition

Process	**Mass Balance (inflow = outflow)**	**Additional Description of Flows**	**Material Levels for Outflows in the Model**
P1: Extraction	$F_{0.1} = F_{1.2} + F_{1.6}$	$F_{1.6}$: Extraction losses.	primary_material
P2: Production	$F_{1.2} = F_{2.3} + F_{2.6}$	$F_{2.6}$: Waste or by-products that occur during production e.g. blast furnace slag.	secondary_material tertiary_material final_material
P3: Finishing	$F_{2.3} + F_{8.3} = F_{3.4} + F_{3.6} + F_{i.3} - F_{e.3}$	$F_{3.4}$: Product in semi-finished state. $F_{3.6}$: Waste or by-product that occur during the finishing process	useful_material
P4: Manufacturing	$F_{3.4} = F_{4.5} + F_{4.8}$	$F_{4.8}$: New scrap generated during manufacturing of metals. It directly goes to recycling.	product new_scrap
P5: Use phase of material stocks	$F_{4.5} = S1 + S2 – F_{5.6}$	$F_{5.6}$: This waste flow includes the end-of-life materials from power sector stocks (S1) and from other stocks (S2) defined as a share of the quantity of generic products.	end_of_life
P6: Waste Collection	$F_{1.6} + F_{2.6} + F_{3.6} + F_{5.6} + F_{8.6} = F_{6.7} + F_{6.9}$	$F_{6.7}$: Total amount of collected recyclable waste. $F_{6.9}$: Waste that is not recycled but treated in other ways. $F_{8.6}$: Recycling losses	total_end_of_life_1/2/3 old_scrap_1/2/3
P7: Waste Preparation	$F_{6.7} = F_{7.8}$	$F_{7.8}$: There are no losses in the waste material but just energy is consumed for preparing recyclable waste for recycling.	new_scrap
P8: Recycling	$F_{4.8} + F_{7.8} = F_{8.3}$	-	final_material
P9: Final Waste Treatment	$F_{6.9} = F_{9.0}$	$F_{9.0}$: Amount of non-recyclable waste	-

S7 Recycling Formulation

Recycling is constrained in the model by using the generic relations formulation.

r= relation, n = node relation, y = year relation, t= time, nl = node location, yv = vintage year, y’ = year active, m=mode,

r= maximum_recycling_limit

relation_activity = 0.9

$$REL_{r,n,y} = \sum_t \left(\left(ACT(scarp\_recovery\_steel)_{nl,t,yv,y\prime,m,}\right) - relation\_activity_{(r,n,y,nl,t,y',m)} \ * \left(ACT(total\_EOL\_steel)_{nl,t,yv,y\prime,m}\right)\right)$$

$$REL_{r,n,y} \leq 0$$

r= minimum_recycling_limit

relation_activity = 0.5

$$REL_{r,n,y} = \sum_t \left(\left(ACT(scarp\_recovery\_steel)_{nl,t,yv,y\prime,m,h}\right) - \mathrm{relation}\_activity_{(r,n,y,nl,t,y',m)} \ * \left(ACT(total\_EOL\_steel)_{nl,t,yv,y\prime,m}\right)\right)$$

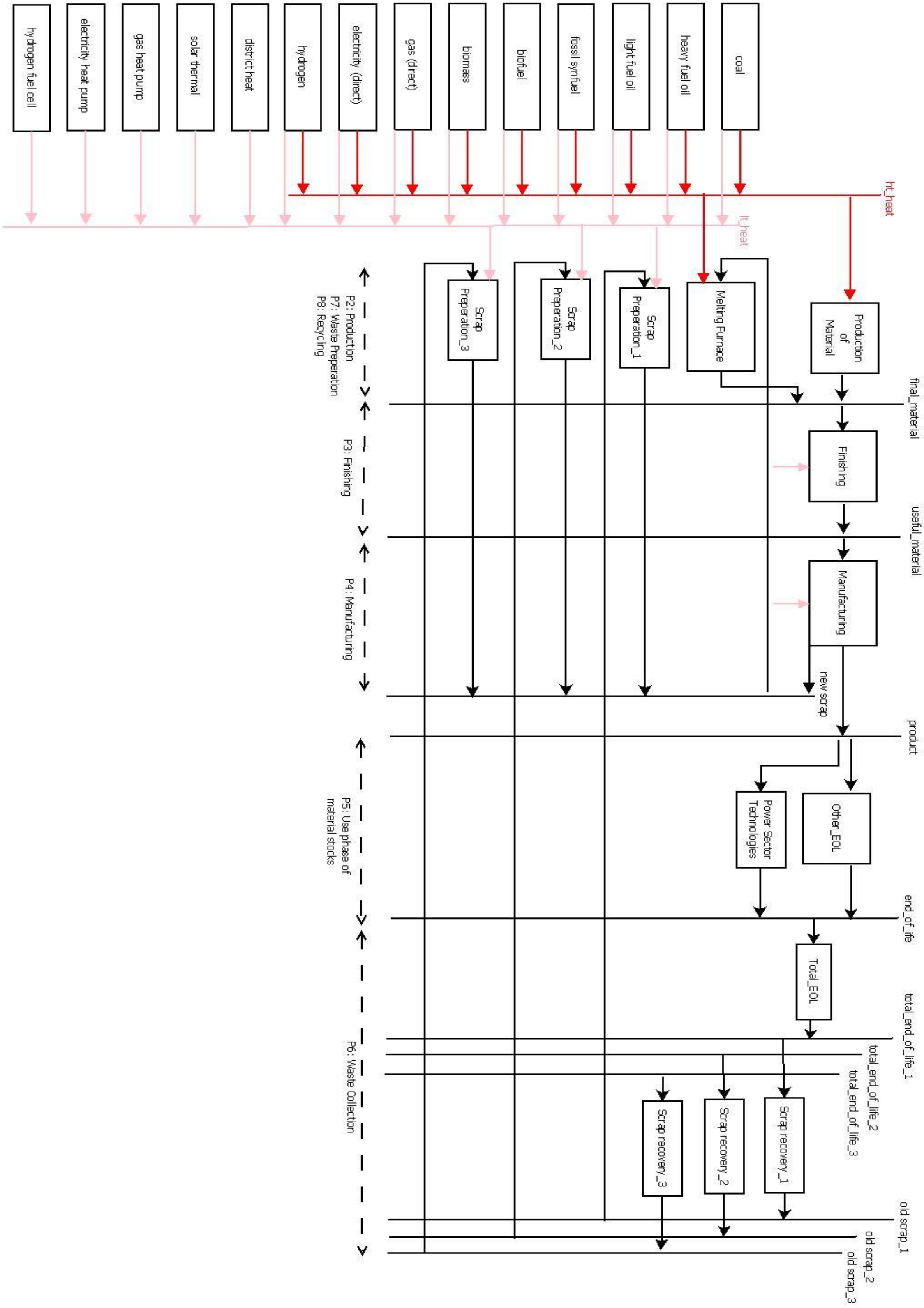
$$REL_{r,n,y} \geq 0$$

For more information on the relation formulation in MESSAGE model refer to: https://docs.messageix.org/en/latest/model/MESSAGE/model_core.html#equation-relation-equivalence

S8 Generic Representation of Material Cycles in MESSAGEix-Materials

Figure S4 shows the generic representation of material cycles in MESSAGEix-Materials by using the reference material system approach. All the thermal energy needs during these steps are satisfied by a set of generic furnace technologies seen at the left of the figure. These technologies allow fuel switching and enable different decarbonization pathways for the high-temperature heat demand in the industry. Below the figure, it is shown how the different processes from Fig. 2 relate to the reference material system.

Figure S4 Generic representation of material cycles in MESSAGEix-Materials.



S9 Validation of the Base Year Model Results

The comparison of the 2020 model values and statistical values is provided in the main text. Table S4 is the collection of data sources that are used as the expected values for 2020 based on different sources.

Table S5, S6 and S7 provide extra details on the comparison of the material stocks from power sector in 2015 in MESSAGEix-Materials with the other literature studies.

Table S4 Sources for data comparison between 2020 model values and statistics per industry sector

Industry Sector	**Final Energy**	**Production**	**Emissions**
Iron and steel	IEA: World Energy Statistics and Balances 2020, IEA [dataset] *The value is the sum of the FLOWs: IRONSTL + TBLASTFUR	World Steel in Figures, World Steel Association, 2020. https://worldsteel.org/wp-content/uploads/2020-World-Steel-in-Figures.pdf	1869 Mt production * 1.42 (emission intensity of iron and steel production in 2020) IEA: Direct CO2 intensity of the iron and steel sector in the Net Zero Scenario, 2010-2030, IEA, Paris https://www.iea.org/data-and-statistics/charts/direct-co2-intensity-of-the-iron-and-steel-sector-in-the-net-zero-scenario-2010-2030
Cement	IEA: Final energy demand of selected heavy industry sectors by fuel, IEA, Paris, https://www.iea.org/data-and-statistics/charts/final-energy-demand-of-selected-heavy-industry-sectors-by-fuel-2019	IEA: Global cement production in the Net Zero Scenario, 2010-2030, IEA, Paris https://www.iea.org/data-and-statistics/charts/global-cement-production-in-the-net-zero-scenario-2010-2030-5260	IEA: CO2 emitted and captured in the cement sector and clinker-to-cement ratio in the Net Zero Scenario: 2015-2030, IEA, Paris, https://www.iea.org/data-and-statistics/charts/co2-emitted-and-captured-in-the-cement-sector-and-clinker-to-cement-ratio-in-the-net-zero-scenario-2015-2030
Aluminium	IEA: World Energy Statistics and Balances, IEA [dataset], https://doi.org/10.1787/data-00512-en, 2019 value	International Aluminum Institute, Global Aluminum Cycle, 2020. https://alucycle.world-aluminium.org/public-access/	IEA, Industry direct CO2 emissions in the Sustainable Development Scenario, 2000-2030, IEA, Paris https://www.iea.org/data-and-statistics/charts/industry-direct-co2-emissions-in-the-sustainable-development-scenario-2000-2030 2018 value

Chemicals	Non-Energy Use: IEA Sankey Diagram: https://www.iea.org/sankey/#?c=World&s=Final%20consumption, 2020 value. Calculation of Energy Use Excluding Feedstock: Share of primary chemicals (47%) * IEA value (IEA Sankey Diagram, 2020 value (covering all chemicals)) Share of primary chemicals in final energy: IEA, ICCA, DECHEMA: Technology Roadmap Energy and GHG Reductions in the Chemical Industry via Catalytic Processes, 2013.	For Ammonia: IEA Ammonia Technology Roadmap, 2020 For High Value Chemicals: IEA The Future of Petrochemicals, 2017 value Methanol: Methanol Institute, 2019 value	IEA: Direct CO2 emissions from primary chemical production in the Net Zero Scenario: 2015-2030, IEA, Paris, https://www.iea.org/data-and-statistics/charts/direct-co2-emissions-from-primary-chemical-production-in-the-net-zero-scenario-2015-2030 Methanol emissions multiplied with the share of the methanol used as feedstock in the industry: 222 * 0.67 = 149 Methanol Institute, 2019

230 **Table S5** Exogenous data on globally installed capacity of electricity generation technologies in 2015 used by MESSAGEix-Materials (this work), Kalt et al. (2021) and Deetman et al. (2021). The three sources use different sets of technology classifications, which were mapped to the common technology set shown in the table below. Data from Deetman et al. (2021) are for the scenario 'BL default'. UNIT: GW

Global capacity 2015 [GW]	MESSAGEix-Materials (this work)	Kalt et al. (2021)	Deetman et al (2021)
Bioenergy & MSW	50.0	106.7	127.3
Coal	1,858.5	1,991.6	1,349.9
Gas	1,621.8	1,561.0	1,200.6
Geothermal	-	11.8	-
Hydro	1,045.1	1,200.0	1,204.2
Nuclear	352.3	343.2	394.8
Oil	464.1	384.1	341.5
Solar CSP	4.7	4.7	4.3
Solar PV	222.6	220.1	175.3
Tidal	-	0.5	-
Wind Offshore	12.0	11.7	8.8
Wind Onshore	425.7	404.9	360.3
Other	-	-	12.6
Sum	6,057.0	6,240.4	5,179.5

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Table S6 Material intensities assumed in MESSAGEix-Materials (this work), Kalt et al. (2021) and Deetman et al. (2021). Where sources report different technology types for one technology category in table above, we calculated the mean for the table categories. For some sources in which regions showed different material intensities. Here we report the minimum and maximum over all regions for MESSAGE-Materials. For Kalt et al. (2021) regional material intensities only differ for the technology Solar PV, which is reported in comment **. To reproduce results, material intensities for each source and technology capacity need to be multiplied at the highest level of granularity. UNIT: ton/GW

Technology	Material	MESSAGEix-Materials max	MESSAGEix-Materials min	Kalt_low	Kalt_med	Kalt_high	Deetman
Bioenergy & MSW	aluminum	1,186	1,166	1,000	2,250	3,500	288
	cement*	54,892	54,369	57,000	81,000	105,000	26,380
	steel	167,599	166,414	70,000	197,500	325,000	39,756
Coal	aluminum	2,246	2,175	200	1,600	3,000	520
	cement*	17,812	17,625	15,000	41,250	67,500	44,739
	steel	41,486	41,120	30,000	65,000	100,000	82,567
Gas	aluminum	1,239	1,211	100	850	1,600	432
	cement*	8,360	8,284	6,750	9,000	11,250	7,102
	steel	19,168	19,034	10,000	30,000	50,000	9,492
Hydro	aluminum	572	572	269	572	876	-
	cement*	787,500	787,500	375,000	787,500	1,200,000	424,893
	steel	45,000	45,000	20,000	45,000	70,000	70,694
Nuclear	aluminum	1,015	965	200	600	1,000	79
	cement*	62,410	61,975	60,000	97,500	135,000	35,285
	steel	75,698	75,254	70,000	90,000	110,000	43,457
Oil	aluminum	1,239	1,211	650	1,000	1,350	600
	cement*	8,360	8,284	7,500	9,375	11,250	32,004
	steel	19,168	19,034	15,000	32,500	50,000	83,499
Solar CSP	aluminum	18,855	13,184	2,600	13,300	24,000	5,500

	cement*	365,484	162,458	15,000	69,750	124,500	202,772
	steel	690,726	483,985	170,000	510,000	850,000	576,236
Solar PV**	aluminum	21,989	16,416	29,150	44,575	60,000	10,176
	cement*	29,301	20,684	11,515	54,542	97,570	-
	steel	69,544	51,530	43,150	106,827	170,503	150,000
Wind Offshore	aluminum	3,654	2,189	784	2,683	4,582	1,438
	cement*	69,651	42,010	-	118,650	237,300	76,370
	steel	494,633	295,361	250,000	400,000	550,000	157,942
Wind Onshore	aluminum	5,263	1,671	784	2,683	4,582	868
	cement*	111,602	35,645	38,100	75,300	112,500	65,093
	steel	355,424	113,489	100,000	142,290	184,580	121,376

* material intensities for concrete from Deetman et al. (2021) and Kalt et al. (2021) were re-calculated to cement intensities at an assumed cement content of 15% in concrete**material intensities of Kalt et al. (2021) are different between regions for Solar PV power plants; the respective minimum and maximum intensities are respectively (t/GW): 18,440/29,150 (aluminum_low), 39,220/44,575 (aluminum_med), 60,000/60,000 (aluminum_high), 25,858/76,767 (concrete_low), 122,481/363,615 (concrete_med), 219,104/650,464 (concrete_high), 19,840/43,150 (steel_low), 55,215/106,827 (steel_med), 90,590/170,503 (steel_high)

Note on data from Deetman et al. (2021):

- From USA/Canada comparison: For Deetman et al., material stock results varied slightly for the year 2015 (0-2.2% per material) in different scenarios, indicating slight deviations of base data. Due to the small differences, we did not follow up on these but instead used the baseline scenario (‘BL’ + ‘default’; see resp. study for details)

Table S7: Data for Fig. 11. Data from Deetman et al. (2021) slightly differ for the base year 2015, the results here represent the scenario ‘BL default’.

unit: Mt	Aluminum					Steel					Cement				
technology	MESSAGEix	Deetman	Kalt_low	Kalt_med	Kalt_high	MESSAGEix	Deetman	Kalt_low	Kalt_med	Kalt_high	MESSAGEix	Deetman	Kalt_low	Kalt_med	Kalt_high
Bioenergy & MSW	0.06	0.06	0.11	0.24	0.37	8.36	7.53	7.47	21.08	34.69	2.73	4.19	6.08	8.65	11.21
Coal	4.11	0.68	0.40	3.19	5.97	76.75	114.20	59.75	129.45	199.16	32.94	71.43	29.87	82.15	134.43
Gas	1.97	0.59	0.16	1.33	2.50	30.95	17.66	15.61	46.83	78.05	13.48	9.41	10.54	14.05	17.56
Hydro	0.6	-	0.32	0.69	1.05	47.03	85.13	24.00	54.00	84.00	823.03	511.66	449.98	944.97	1,439.95
Nuclear	0.34	0.03	0.07	0.21	0.34	26.60	17.16	24.03	30.89	37.75	21.89	13.93	20.59	33.46	46.33
Oil	0.57	0.20	0.25	0.38	0.52	8.87	24.89	5.76	12.48	19.21	3.86	10.93	2.88	3.60	4.32
Solar CSP	0.07	0.02	0.01	0.06	0.11	2.36	2.49	0.81	2.42	4.04	0.92	0.88	0.07	0.33	0.59
Solar PV	4.12	1.78	5.16	9.18	13.21	12.76	26.29	6.77	17.48	28.18	5.12	-	1.64	7.77	13.91
Wind Offshore	0.03	0.01	0.01	0.03	0.05	4.06	1.38	2.93	4.69	6.44	0.57	0.67	-	1.39	2.78
Wind Onshore	0.91	0.31	0.32	1.09	1.86	62.43	43.73	40.49	57.61	74.73	19.60	23.45	15.43	30.49	45.55
Geothermal	-	-	0.04	0.06	0.08	-	-	0.18	1.27	2.36	-	-	0.21	0.21	0.21
Tidal	-	-	0.00	0.00	0.00	-	-	0.01	0.02	0.04	-	-	0.19	0.40	0.62

Other	-	0.05	-	-	-	-	2.72	-	-	-	-	1.94	-	-	-

S10 Technology Diffusion Constraints

MESSAGE model tracks investments by vintage, an important feature to represent the inertia in the energy system due to its long-lived capital stock. In case of shocks (e.g., introduction of stringent climate policy), it is however possible to prematurely retire existing capital stock such as power plants or other energy conversion technologies and switch to more suitable alternatives.

An important factor in this context that influences technology adoption in MESSAGE*ix* are technology diffusion constraints. Technology diffusion in MESSAGE*ix* is determined by dynamic constraints that relate the construction of a technology added or the activity (level of production) of a technology in a period *t* to construction or the activity in the previous period *t-1*. While limiting the possibility of flip-flop behavior as is frequently observed in unconstrained Linear Programming (LP) models such as MESSAGE*ix*, a drawback of such hard growth constraints is that the relative advantage of some technology over another technology might not be taken into account and therefore even for very competitive technologies, no rapid acceleration of technology diffusion might not be possible. In response to this limitation, so called flexible or soft dynamic constraints have been introduced into MESSAGE. These allow faster technology diffusion at additional costs and therefore generate additional model flexibility while still reducing the flip-flop behavior and sudden penetration of technologies. For example, a value of 0.05 for the growth_activity_up parameter sets an upper bound of 1+0.05 = 105% activity in one year relative to the activity in the preceding year. In a period with duration 5 years, the activity in the representative year is bounded at (1.05)^5 = 128% of the activity in the representative year of the preceding period.

More details on the formulation and the parameters can be found here: https://docs.messageix.org/en/latest/model/MESSAGE/model_core.html#dynamic-constraints. The constraints in this section specify dynamic upper and lower bounds on new capacity and activity. These can be used to model limits on market penetration and/or rates of expansion or phase-out of a technology.

The parametrization that is used for this model version can be found in the data section of the model repository for each industry in the separate folders: https://github.com/iiasa/message-ix-models/tree/update_steel_rebase/message_ix_models/data/material.

S11 Additional Graphs on Energy System Transition, End-Use Sectors and Technologies

Figure S5 Primary Energy, Final Energy by end-use sector, Direct CO2 Emissions by end-use sector respectively

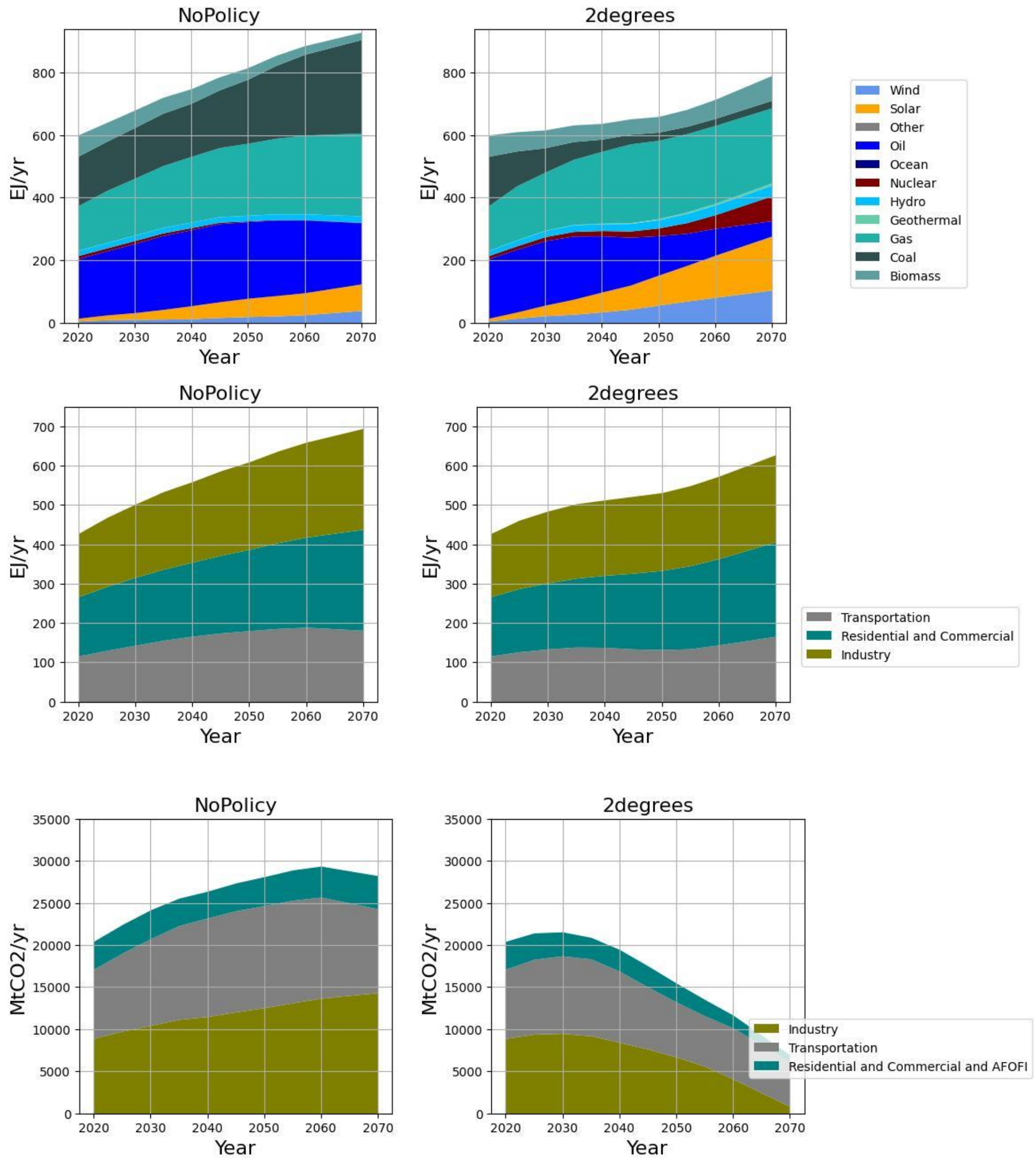


Figure S6 Final Energy Mix of Other Sector

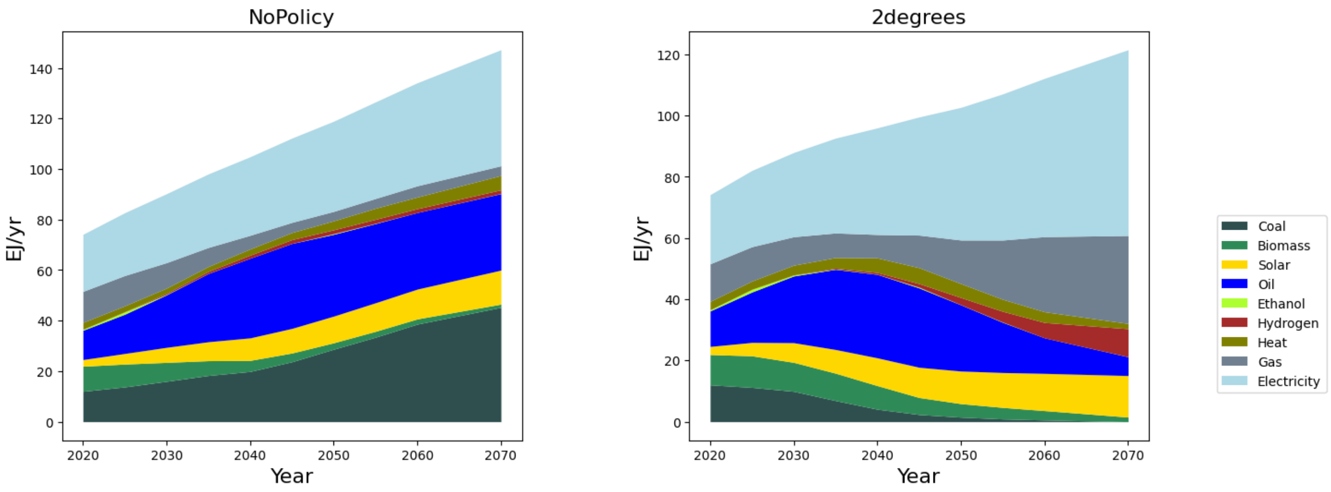
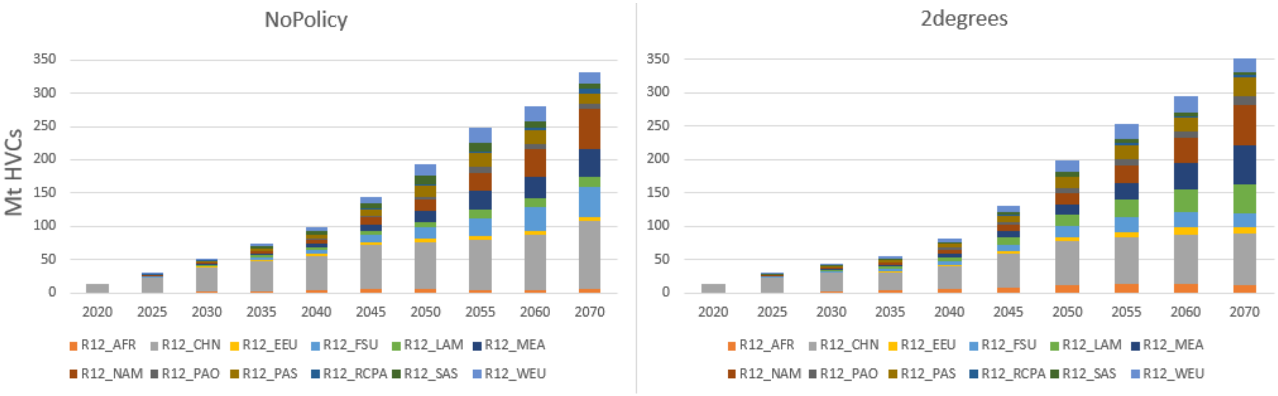
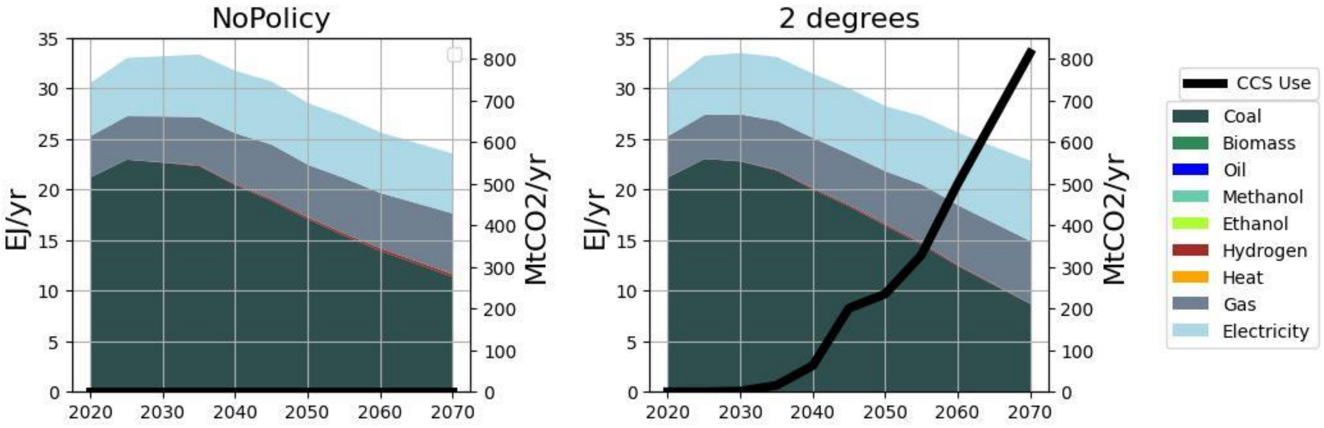


Figure S7 Regional MTO Use



S12 Iron and Steel Industry

Figure S8 Final Energy and CCS Usage



S13 CCS Usage in Cement Industry

Figure S9 shows the comparison of CCS usage in cement industry in two different climate policy scenarios, 2 degrees and High Carbon Price. The High Carbon Price is a scenario that is used to push the model to its limits to see the highest potential of technological deployments within the feasible model solution. The carbon price in this scenario starts with around 300 USD/MtCO2 in 2025 and keeps increasing with a 5% discount rate. In such a setting, it is seen that CCS deployment for cement can already start around 2025 and the model keeps using the technology increasingly in the coming years as much as the technological diffusion constraints in the model allow the scale up. The details on technology diffusion constraints are described in Supplementary S10. In 2 degrees scenario, CCS option becomes more cost optimum system-wide only after there are CCS cost reductions in the model input which is in 2050. After that the model catches up with the high carbon price scenario in 2070. Figure S10 shows the carbon price difference between the two scenarios. The shaded area between the 2 degrees and High Carbon Price scenario is the option space where higher carbon prices and stricter climate policy can generate higher CCS deployments in cement industry in the early years as a result of the techno-economic costs provided as input to the model.

Figure S9 CCS Use in Cement Industry, 2 degrees and High Carbon Price Scenarios

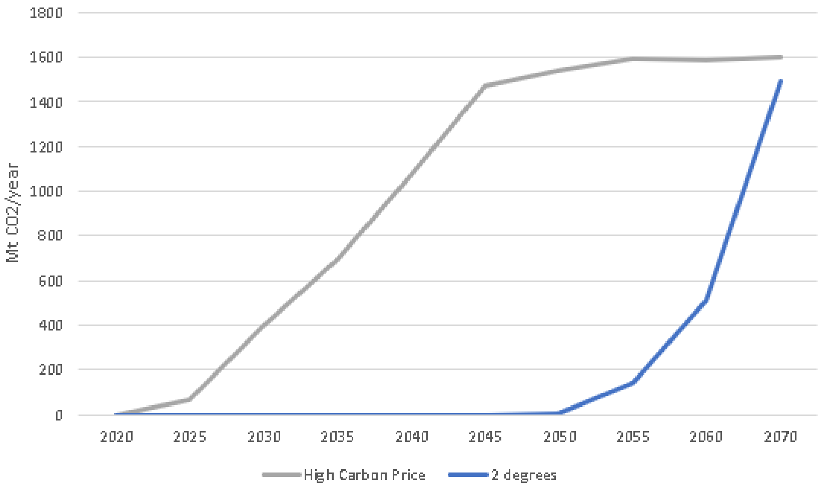
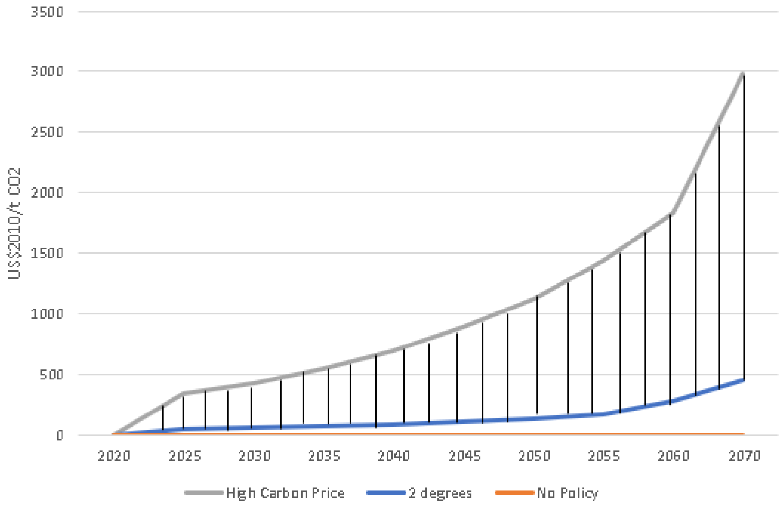


Figure S10 Carbon Prices in No Policy, 2 degrees and High Carbon Price Scenarios



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