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# MESSAGEix-Materials v1.0.0: Representation of Material Flows and Stocks in an Integrated Assessment Model

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**Abstract.** Extracting and processing raw materials into products in industry is a substantial source of CO2 emissions, which is currently lacking process detail in many integrated assessment models (IAMs). To broaden the space of climate change mitigation options and to include circular economy and material efficiency measures in IAM scenario analysis, we develop MESSAGEix-Materials module representing material flows and stocks within the MESSAGEix-GLOBIOM IAM framework. With the development of MESSAGEix-Materials, we provide a fully open-source model that can assess different industry decarbonization options under various climate targets for the most energy and emissions-intensive industries: Aluminium, iron and steel, cement, and petrochemicals. We illustrate the model's operation with a baseline and mitigation (2 degrees) scenario setup and validate base year results for 2020 against historical datasets. We also discuss the industry decarbonization pathways and material stocks of the electricity generation technologies resulting from the new model features.

## 1 Introduction

Extracting and processing raw materials into products which are used in various end-use sectors such as transportation, residential and commercial buildings, infrastructure, or consumer goods is a substantial source of CO2 and greenhouse gases (GHG) emissions. Direct and indirect CO2 emissions from industries constitute 35% of global GHG emissions (Lamb et al., 2021) and industry constitute 37% (157 EJ) of the global total final energy use in 2018 (IEA,2023c). Around 70% of the industrial CO2 emissions and 50% of the final energy consumption are due to the production of bulk materials such as aluminium, cement, iron and steel, and petrochemicals (IEA, 2021c). Therefore, options on how to decarbonize these industries via energy- and material efficiency as well as demand-side measures are increasingly investigated (Watari et al., 2022, Lopez et al., 2023, Bhaskar et al., 2020). Understanding the potentials of these mitigation measures for reducing GHG emissions then requires model-based assessments of the entire life cycle of materials, from raw material extraction, industrial processing, to the use-phase of product stocks, as well as waste management, recycling and end-of-life treatment options.

Integrated Assessment Models (IAMs) have been used to generate scenarios for assessing energy and industry transformation for limiting climate change. However, recent reviews showed that many IAMs often lack the granularity, resolution, and framework to fully depict material flows and stocks (Bataille et al., 2021; Pauliuk et al., 2017; Stern, 2011). Many IAMs either omit physical material supply and demand, or model those in a simplified manner by directly relating material flows to economic indicators such as GDP (Pauliuk et al., 2017). Connecting material flows with end-use demand would however enable modelling such cross-sectoral interactions among material stocks and flows, and energy demand and GHG emissions and only very few models cover the entire life cycle of material flows and stocks in a physically consistent manner (Wiedenhofer et al., 2023). Partial equilibrium IAMs are technology-rich optimization models built on thermodynamic consistency for their respective sector such as energy system. Only recently, partial equilibrium IAMs started to represent material flows and stocks and their energy and emissions-intensive production processes. For example, Stegmann et al (2022) uses IMAGE to represent plastics, van Sluisveld et al (2021) to represent iron and steel, cement, chemicals, paper and pulp and Deetman et al (2021), (2020), (2018) for specific end-use sectors such as electricity, buildings, vehicles and appliances. Other partial equilibrium IAMs such as COFFE, POLES and PROMETHUS (Rochedo et al., 2016; Després et al., 2018; Fragkos et al., 2015) include iron and steel, cement, and chemicals.

Herein, we present MESSAGEix-Materials module, which aims to model the lifecycle of energy-intensive materials starting from raw material extraction, industrial processing, their accumulation as material stocks for various end-uses, to end-of-life waste flows and recycling within the MESSAGEix-GLOBIOM integrated assessment modeling framework (Krey et al., 2020). We develop the module based on a conceptual framework that integrates the traditions of energy systems modeling with economy-wide material flow analysis. With this development, we provide a fully open-source model and its associated techno-economic data which can be used to assess different industry decarbonization options under various climate targets for the most energy- and emissions-intensive industries: iron and steel, cement, aluminium and petrochemicals.

MESSAGEix-Materials is operational within the global partial equilibrium MESSAGEix-GLOBIOM model that is based on the MESSAGE*ix* modelling framework (Huppmann et al., 2019) which can also incorporate macro-economic feedback using a stylized computable general equilibrium model, MACRO. The energy systems optimization model MESSAGE (Model for Energy Supply Strategy Alternatives and their General Environmental Impact) and the land-use model GLOBIOM (GLObal BIOsphere Model) (IIASA-IBF, 2023; Havlík et al., 2014) are the central components of the framework. Based on its scenarios GLOBIOM is linked to MESSAGE as a parametric land-use emulator (Fricko et al., 2017). MESSAGE is a linear programming (LP) cost minimization energy engineering model with global coverage and perfect foresight as solving method. MESSAGEix-GLOBIOM provides a framework for representing a reference energy system with a full set of available energy conversion technologies from resource extraction, imports and exports, conversion, transport, and distribution, to the provision of energy end-use services such as light, space conditioning, industrial production processes, and transportation. More details about the integration of MESSAGEix-Materials to MESSAGEix modeling framework are explained in Sect 2.4.

As a system engineering optimization model, MESSAGE*ix* is primarily used for medium- to long-term energy system planning, energy policy analysis, and scenario development (Huppmann et al., 2019; Messner and Strubegger, 1995). The model is designed to formulate and evaluate alternative energy supply strategies consonant with user-defined constraints such as limits on new investment, fuel availability, trade, environmental regulations and policies as well as diffusion rates of new technologies (Gidden et al., 2023; Guo et al., 2022; Zhou et al., 2019). Environmental aspects can be analyzed by accounting, and if necessary, limiting the amounts of pollutants emitted by various technologies at various steps in energy supply. This helps to evaluate the impact of environmental regulations on energy system development. The principal results comprise, among others, estimates of technology-specific multi-sector response strategies for specific climate stabilization targets. By doing so, the model identifies the least-cost portfolio of mitigation technologies. The choice of individual mitigation options across greenhouse gases and sectors is driven by the relative economics of the abatement measures, assuming full temporal and spatial flexibility (i.e., emissions-reduction measures are assumed to occur when and where they are cheapest to implement).

However so far, MESSAGEix-GLOBIOM only contains a simplified representation of the industry sector by distinguishing three industrial energy demand categories: thermal, specific, and feedstock. Thermal demand, i.e., heat at different temperature levels, can be supplied by a variety of different energy carriers while specific demand requires electricity (or a decentralized technology to convert other energy carriers to electricity). Industrial production processes are not explicitly modeled but for example the amount of cement production is linked to industrial activity (more specifically the industrial thermal demand in MESSAGEix) and the associated CO2 emissions from the calcination process are accounted for explicitly (Krey et al., 2020). However, the current representation of industrial energy demand is solely derived via GDP, which is not biophysically consistent as there is no link between material flows, accumulated stocks and the related energy.

The MESSAGEix-Materials module presented herein addresses this simplified industry sector representation and develops a consistent representation of material extraction, industrial production and processing technologies, together with the relevant techno-economic data for the chosen industries. This enables explicitly representing the primary and secondary material flows occurring in industrial processes and, the resulting GHG emissions, opening the way for modelling materials-oriented climate change mitigation strategies. For the industries mentioned above, a set of low-carbon technologies in addition to the conventional technology options, are represented including recycling for metals. Because capital formation is a major driver of material demand and GHG emissions (Hertwich, 2021), we extend the MESSAGEix model formulation (Huppmann et al., 2019) to also explicitly model material flows from the existing technologies in the model. We demonstrate the functionality

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of the new model formulation for the case of electricity generation technologies to allow endogenizing material demand and end-of-life materials from building up and transforming the infrastructure for these technologies. This formulation can also be used for other technologies in the model such as machinery in industry, or vehicles in the transportation sector when there is data available. One major challenge in developing a module that aims to have a comprehensive representation of the industry sector is gathering techno-economic data, especially regional differences. Table S1 in supplementary material lists all the data sources for different industries that were used in building up this module for 12 model regions. The details about model regions are seen in Table S2 in supplementary material. In that sense, we also provide a collection of techno-economic data sources with the open-source release of the module.

This version 1.0.0 of the MESSAGEix-Materials module is the first step of an ongoing development process which aims to improve the overall representation of material stocks and flows, industry sectors and their link to end-use demand, ultimately to represent the relations between societies' demand for service provisioning (e.g. building floorspace), the required material production and processing, as well as the associated energy and GHG emissions for industrial production and product stock operation ('stock-flow-service' nexus; Haberl et al., 2017).

In the remainder of this paper, Sect. 2 provides an overview of the MESSAGEix-Materials module including integrative system definition (Sect. 2.1), the sector-specific representation for iron and steel, cement, aluminium, and petrochemicals (Sect. 2.2), the demand side representation in the module (Sect. 2.3), and the modeling approach (Sect. 2.4). Section 3 presents the results from MESSAGEix-Materials while Sect. 4 is a discussion of these results including limitations and further plans for development.

## 2 Model Description

### 2.1 Integrative System Definition

In traditional energy systems modelling, the primary focus lies on the energy commodities that serve as inputs to various socio-economic processes and their implications for greenhouse gas emissions. Energy commodities are measured in energy units and traced from the extraction of primary energy carriers, along transformation processes to useful energy. Any energy losses along the supply-chain and in the use phase, e.g., waste heat, typically goes unreported as it dissipates, but could be reconstructed as residuals from the tracked energy flows. At the same time, the flow of carbon and other GHGs is tracked in a thermodynamically correct, mass-balanced manner, because a key objective of energy systems models is to analyze GHG emission reduction strategies (Dodds et al., 2015; Herbst et al., 2012).

To address the mitigation potentials of materials-oriented strategies such as the circular economy and material efficiency, it becomes necessary to expand the scope of this energy-focused model towards fully covering material cycles and the dynamics of material stocks (Pauliuk et al., 2017). For this purpose, we draw on the field of industrial ecology, specifically Material Flow Analysis (MFA), which is widely used in the context of resource- and waste management (Graedel, 2019), as well as to quantify economy-wide resource use in accordance with system boundaries of the System of National Accounts (Eisenmenger et al., 2020; Krausmann et al., 2017). MFA is based on the concept of social metabolism, conceptualizing society as socio-ecological 'organisms', requiring inputs of material and energy to build up, sustain and reproduce their biophysical stocks of people, livestock and non-living material stocks, thereby producing waste and emissions (Fischer-Kowalski, 1998; Gerber and Scheidel, 2018). In recent years, dynamic MFA is increasingly used to implement a systemic, economy-wide perspective and to simulate stock/demand- or inflow/supply-driven scenarios, assessing technical/physical potentials and limits of material efficiency and circular economy strategies, e.g., lifetime extension, lightweighting, reuse, recycling, downsizing (Hertwich et al., 2019; Worrell et al., 2016; Wiedenhofer et al., 2019; Lanau et al., 2019). The conservation of mass is the fundamental principle in MFA, which entails accounting for all by-products and waste flows occurring along material cycles from extraction to industrial processing, use as stocks, and end-of-life material flows (Graedel, 2019). This means that all material inputs into a system over a certain time period have to be equal to all outputs over the same period, plus/minus stock changes. A clear systems definition covering system boundaries, as well as processes and stocks and flows is indispensable for ensuring compliance with the mass-balance principle. A general material cycle system definition in economy-wide material flow analysis and additional information about the methodology can be seen in Fig. S3 in supplementary.

Combining energy systems modeling with economy-wide material flow analysis requires us to focus on aspects that were not considered essential in traditional energy systems modeling. Therefore, we created a conceptual framework that outlines the targeted system boundaries of MESSAGEix-Materials within the physical earth system and the socio-economic system as commonly defined in the System of National Accounts. In the conceptualization of the model and the definition of system boundaries, we draw on the latest literature and developments in economy-wide material and energy flow analysis (Plank et al., 2022; Krausmann et al., 2020; Pauliuk and Hertwich, 2015). Version 1.0.0 of MESSAGEix-Materials is a proof-of-concept implementation of the conceptual framework presented in Fig. 1. The figure shows the modeling of industrial and end-use processes denoted by P where material flows and stocks for cement, aluminium, steel and primary chemicals (ethylene, propylene, benzene, toluene, xylene) occur. More details about the material flows, the mass balance equations and the corresponding material levels that are used to represent the flows in MESSAGEix-Materials in line with the energy systems modelling (see Sect. 2.2) are described in supplementary Table S4.

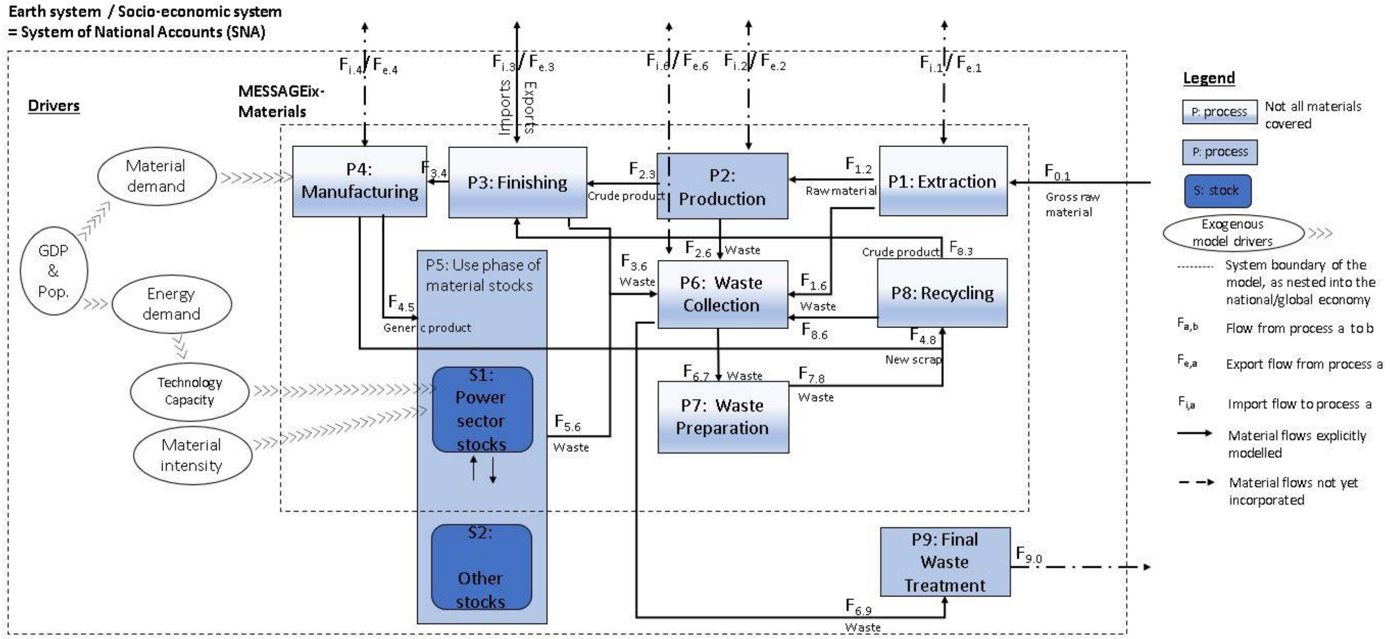

**Figure 1: Generic representation of material flows and stocks in MESSAGEix-Materials.**

Since in MESSAGEix-Materials, material demand for products drives industrial production of materials accumulating as stocks similar to the approach in other integrated assessment model literature (Deetman et al., 2021), the drivers of the model are presented on the left side. As a result of the exogenous demands the quantity of materials that needs to be produced is determined which then determines the quantity of the extraction. Raw materials extraction process (P1), as defined in economy-wide material flow accounting (Eurostat, 2018; United Nations Environment Programme, 2023) represents the process of extracting natural resources such as non-metallic minerals, ores, biomass, and fossil energy carriers from natural deposits, which are then further processed and traded (Plank et al., 2022). The model offers an example representation of detailed extraction processes through its implementation of the extraction of fossil fuels[1] such as coal, gas, and oil, which are subsequently utilized as feedstocks in the chemical industry. Representation considers factors like the physical, technical and economic resource availability, costs at which raw material can be brought to the surface and the losses from “resource” to “primary” energy level. Following the extraction phase, the raw materials move on to the production stage (P2), where detailed production technologies specific to each industry are explicitly represented. In this stage, the material and energy inputs related to the production process are provided together with production costs and emission factors. A more comprehensive explanation of this phase can be found in Sect. 2.2 for each material. Subsequently, there's the Finishing (P3) and Manufacturing (P4) phase that produces generic products that then enter the use phase (P5). Trade is only represented for semi-finished goods for

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[1] https://docs.messageix.org/projects/global/en/latest/energy/resource/fossilfuel.html

steel, aluminium and chemicals as part of P3. During manufacturing, a fixed percentage of new scrap is formed in case of metals. This type of scrap requires less preparation before recycling and has higher quality as it is the direct product of the manufacturing. It is usually directly used within the manufacturing without going through the market first, unlike the old scrap which is formed at the end of the life cycle of metals. Drivers of the use phase (P5) is explained in more detail below. Once products reach their end of lifetime, they are collected in Waste Collection (P6) and further distributed either for Recycling (P8) which is preceded by a preparation phase, Waste Preparation (P7) or for final disposal and treatment in Final Waste Treatment (P9) and not recycled.

For aluminium and steel, waste (for metals known as old scrap) is distinguished based on the scrap quality, forming a scrap supply curve with three different levels 1/2/3, 1 being the highest quality of scrap and 3 being the lowest. Different initial designs and final use conditions of a product determine the ease of recycling which is reflected in different scrap qualities in the model. Based on a simple supply curve logic, different quality scraps are available in different quantities, medium quality scrap (2) being available the most. A minimum recycling rate can be specified at the Waste Collection (P6) for steel and aluminium either based on historical recycling rates or regulatory policies in different regions. The recycling rate in the model can be higher than the specified minimum depending on the economic attractiveness of the recycling options compared to primary material production. In addition, there is a maximum recycling rate imposed to represent the limitations on recycling (e.g., contamination in steel). The energy intensity and costs for the recycling process increase during the Waste Preparation (P7) as the scrap quality degrades. After preparation, scrap is sent to Recycling (P8) where it is turned into final materials to be used in the Finishing & Manufacturing (P3 and P4) again. During this process, recycling losses (F8.6) are also considered. It is assumed that the recycled materials have the same quality after the recycling process. All the old scrap that is collected in the waste collection stage (F7.8) is used in the recycling assuming scrap availability and collection rate are the main bottlenecks of the recycling process. Final waste treatment such as landfilling, incineration or waste-to-energy are defined as being outside of the system boundaries of the model. To maintain mass balance, all material flows including waste in various stages (F1.6, F2.6, F3.6, F5.6, F8.6) can be tracked at each stage by adding relevant reporting variables to the reporting code.

The calculation of material stocks in the model version 1.0.0 differs between the power sector which is composed of electricity generation technologies, and other sectors, as outlined in Fig. 1, block P5 as S1 and S2. In the case of the power sector, the capacity of electricity generation technologies in the cost-minimization problem is determined by electricity demand, which is driven by energy service demands which themselves are linked to population and GDP, and competitiveness of different fuel-to-service routes. The required material stocks and their associated material flows are then endogenously determined by the modelling framework for the electricity generation technologies. For example, material stock accumulation of the power sector (S1) is determined by the multiplication of the newly built electricity generation technology capacities (e.g. solar panels, hydropower facilities, fossil fuelled power plants etc.) and the exogenous material intensities of those (see Sect. 2.3.1). Further details on the modified model formulation to enable this calculation can be found in Sect. 2.4. Material flows not related to the power sector (S2) are determined exogenously in a highly aggregated manner by using GDP and population driven demand quantities for products. The stocks then can be calculated based on this flow and GDP correlation as described next. A portion of the manufactured products goes into use-phase (P5) and becomes waste not based on the lifetimes but based on ratios used in the model, while the remainder can be considered as stock. For a certain material, that waste ratio is determined by using what is reported in the statistics. This ratio is precisely calculated by dividing overall waste quantity (from both long- and short-lived products) to the total production quantity in the base year. This base year ratio is used in all years in the model to determine the waste quantity.

Because version 1.0.0 of MESSAGEix-Materials is a proof-of-concept implementation of the novel conceptual framework described above, there are some deviations how the implementation of the general system definition shown in Fig. 1 is achieved for specific materials and industries which are discussed in Sect. 2.2. For the next versions, we aim to achieve a comprehensive, economy-wide operationalization across all materials and end-uses. These deviations stem from the strategic decision to initially prioritize the representation of the most energy- and emissions-intensive processes first. These deviations are: First, for non-metallic minerals and metals, we do not fully cover the raw material extraction and mining phase (P1). Specifically, we exclude the detailed representation of economic costs, energy use and physical waste and losses during raw material extraction of gross ores. For steel, we only use the quantity of the iron ore required to produce one unit of steel in the production process. For aluminium, the model does not account for bauxite extraction as input to the system but starts with the most energy and emissions-intensive phase of production which is smelting, with alumina as the input material. For cement, the quantity of limestone to produce one unit of clinker is included in the model as the main material input to cement production. However, other non-metallic minerals like clay, shale, or sand and gravel, that are mixed with cement to form concrete, are excluded. Secondly, the current approach only explicitly models product lifetimes for electricity generation technologies, while all other material stock end-uses are determined based on simplified and aggregated approach as described above. It is important to note that, due to lack of data for the multitude of chemicals used nowadays, there is no product end-use detail and therefore no stocks are represented explicitly as those chemicals are contained in various products. The only exception is nitrogen fertilizer, which is modelled explicitly, but which does not accumulate as stock but is dissipated to the environment on purpose. Thirdly, in the waste collection (P6), preparation (P7) and recycling (P8) phases, only metals are modelled, while end-of-life flows of chemicals and cement is not represented as recycling/downcycling of cement currently occurs only at very low levels (Cao et al., 2017). Finally, in this version of the model, Final Waste Treatment (P9) technologies, costs and mass-balances are not included.

Despite these derivations from the general system definition, MESSAGEix-Materials version 1.0.0 serves as the foundation for future work incorporating further material flows and product stocks as needed for specific research questions related to a particular sector and/or material. This version of the model is therefore introduced as a proof-of-concept, which exemplifies how energy systems modeling and economy-wide material flow analysis can be integrated to represent material stocks and flows and their energy requirements and GHG emissions implications. As next steps, the extraction and mining phase (P1) can be represented in detail for those other materials similarly as for fossil fuels[1.] In addition, explicit dynamic stock-flow implementations as for electricity generation technologies can be introduced to the model to increase the endogenous coverage of other material stocks such as buildings, infrastructure or vehicles. Regarding the end-of-life, it is possible to extend cement and chemical flows to P6, P7 and P8 by following the same structure as other materials. For chemicals, plastics need to be represented as an explicit commodity in the model for a better representation of waste treatment options.

### 2.2 Material Supply and Processing in Reference Energy and Material System

MESSAGEix-Materials includes the explicit representation of technologies and processes from four key energy/emissions-intensive material industries: Steel, cement, aluminium, and petrochemicals. The life cycle representation of different material industries in the model follows a generic structure as shown in the form of a *Reference Material System*, analogue to the common *Reference Energy System* representation used in energy system modeling (Beller, 1976) and is customized based on the process-specific differences between industries. A generic reference material system diagram for the model can be seen in supplementary Fig. S5. Different than Fig. 1, these series of figures that are used through Sect 2.2 provide information on explicitly how the processes are modelled in MESSAGEix-Materials for a specific industry. Similar to the representation of energy commodities in energy engineering models such as MESSAGEix, depending on the stage of the material in its lifecycle, materials exist in different levels *primary_material, secondary_material, tertiary_material, final_material, useful_material, product, end_of_life, old_scrap 1/2/3*. Table S4 in supplementary shows how these levels are connected to the system boundaries and processes from Fig. 1.

In Figures 2, 3 and 4, the use-phase and end-of-life phase of the resulting products is represented endogenously for the power sector while the rest is represented in the generic category 'Other_EOL'. The additional step 'Total_EOL' collects all the available waste at the total_end_of_life level. Below the specific representation per industry sector is explained.

### 2.2.1 Iron and Steel

The iron and steel sector has one of the highest carbon footprints among all bulk-material industries. Globally, the sector makes up 25% of the total direct industry CO2 emissions with 2.1 Gt in 2018 (IEA, 2020c). Crude steel production in 2020 amounted to 1880 Mt (Statista, 2023) and the final energy use was 37 EJ in 2020 responsible for 24% of the final energy demand of the industry and 8% of the global final energy demand (IEA, 2020c). Steel is used most notably in the construction sector to build buildings and infrastructure as well as to produce machinery (Pauliuk et al., 2013). In addition, it will also be an important material for the energy transition, being used in low-carbon technologies such as solar panels, wind turbines, hydropower, and electric vehicles. Global steel demand has increased more than threefold since the 1970s as the rapid urbanization and buildup of infrastructure continues (IEA, 2020c).

Steel is produced mainly through two routes. The more dominant practice is through *blast furnaces*, which produce pig iron from iron ore, and *basic oxygen furnaces*, which converts molten pig iron into steel by blowing pure oxygen into the charge (BF-BOF process). There is a competing process called DRI-EAF routes (*direct reduction iron* and *electric arc furnace*), which goes through direct reduction of iron ore without melting it and uses electricity to smelt the charge and make raw steel. This process using EAF (not necessarily with DRI) has a lower energy use than BF-BOF which involves energy-intensive processing of raw materials. Also, EAF can be installed in smaller units for different market sizes and can be more economical than BF-BOF because it can rely fully on scrap metal as its input material with the possibility to vary the input mix based on the market situation. While some of the countries with large steel-making capacities like the USA, India, and Italy rely heavily on the EAF steel-making process, still the BF-BOF is the dominating technology globally, especially in China, which produces more than half of steel globally. China produces 90% of its steel from BF-BOF (World Steel Association, 2020).

The MESSAGEix-Materials model implements these two routes, while also considering old scrap material inputs back into the material production process. The modeled process for the BF-BOF route includes the raw material preparation step, which involves coke oven and sinter/pellet plants. Figure 2 below shows the reference material system for iron and steel.

Iron and steel was the world's 9th most traded product in 2021 (OEC, 2023). International trade of iron and steel is also an essential component to understand the technological changes and supply chain dynamics from raw materials to finished products.  In the model, trade is represented at the useful_material level which delivers semi-finished steel after the finishing process. Regions can import and export semi-finished iron and steel from a global trade pool.

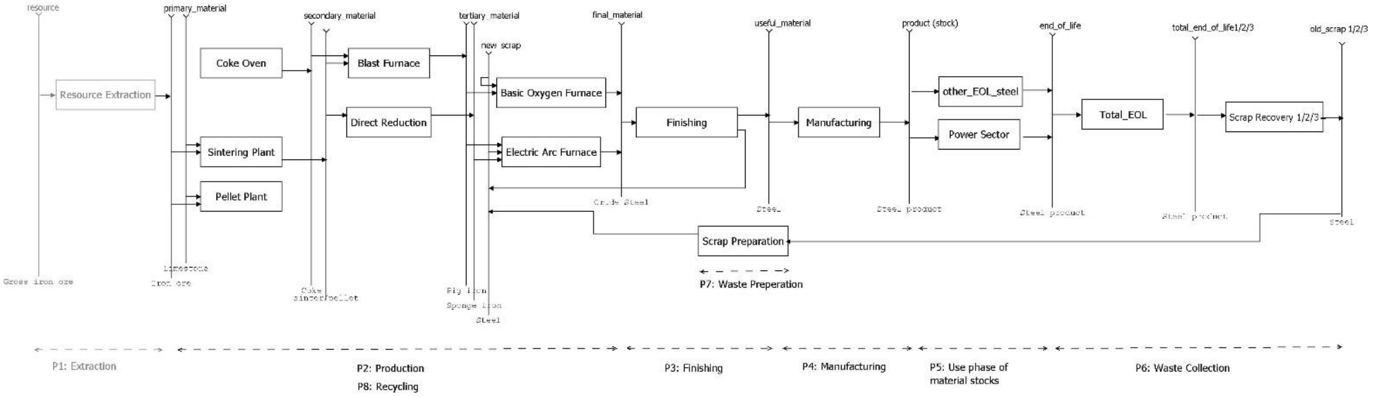

**Figure 2: Reference Material System for iron and steel.**

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### 2.2.2 Aluminium

The aluminium industry is mostly known for its indirect emissions due to high electricity needs of the industrial processes. The sector is directly responsible for almost 200 Mt of direct CO2 emissions in 2018 (2.3% of the total industry emissions) and the number goes up to 1 Gt of CO2 if the emissions from electricity consumption is included (IEA, 2023a). Production amounts to 94 Mt in 2018 (IAI, 2018; Idoine et al., 2023) and final energy use is around 5 EJ in 2020 (3% of the total industry final energy) (IEA, 2023b).

Aluminium is one of the non-ferrous metals that is widely used in the end-use sectors such as transportation, buildings, and consumer goods. The contemporary global aluminium stock in use has reached about 10% of that in known bauxite reserves and still no clear signs of saturation can yet be observed (Liu and Müller, 2013).  In the context of the transformation to low carbon energy system, it plays an important role for strategies such as lightweighting in the transport sector or for grid infrastructure expansion as a result of increasing renewable energy technologies (Kalt et al., 2021; Deetman et al., 2021).

The production process for aluminium consists of two main steps: refining and smelting. Refining is the step where the extracted bauxite mineral is converted to an intermediate material, alumina. This process is not explicitly represented in the model, as the decarbonization potential mostly comes from smelting with its 78% share of energy consumption within the whole production process (IEA, 2009). In the model, the first step of the production process is smelting which takes alumina as input from an unlimited supply with a relevant variable cost. Smelting is performed by two commercially available technology options; Prebake and Soderberg. Both technologies require significant electricity input which makes the primary energy intensity and indirect emissions very much dependent on the energy mix of a certain region. The liquid aluminium is then converted to the final product by following the finishing and manufacturing processes.

The melting furnace and scrap preparation technologies enable the usage of old and new scrap as an alternative production path to smelting with significantly less energy requirement. Figure 3 below shows the production processes for aluminium as represented in the model. The trade of aluminium is represented at the useful_material level which has the semi-finished aluminium after the finishing process. Regions can import and export semi-finished aluminium at the useful_material level from a global trade pool.

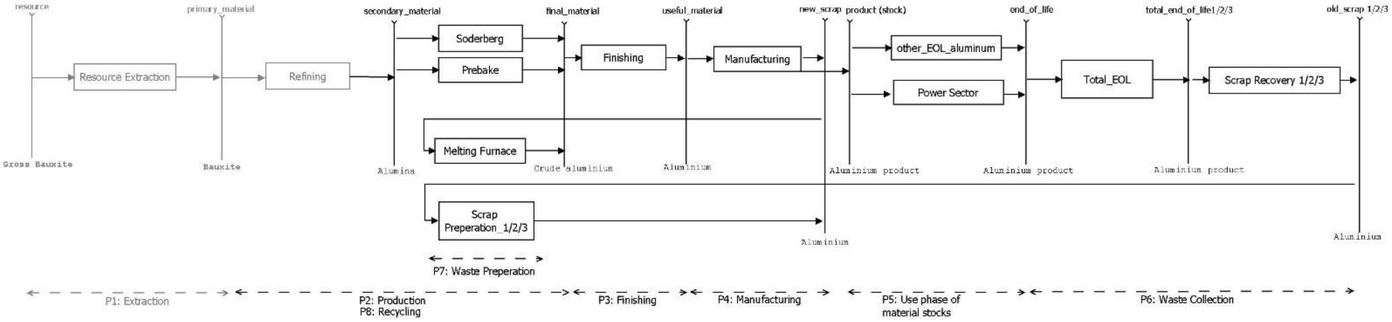

**Figure 3: Reference Material System for aluminium.**

### 2.2.3 Cement

While cement production consumes less energy than steelmaking, it is one of the most emission-intensive industries amounting to 2.3 Gt CO2 in 2018 around 27% of total industry emissions (IEA, 2020b). In 2020, cement production amounted to 4100 Mt/year, with a global thermal energy use intensity of 3.55 GJ/t (IEA, 2023d). Cement is widely used in buildings and infrastructure development such as bridges or dams and due to ongoing urbanization and increasing affluence around the world, the demand for cement is expected to increase. (Cao et al., 2017) About 60% of the emissions from cement production come out of a chemical process called calcination (Kermeli, 2016). Calcination is a process to remove carbon as carbon dioxide from limestone (calcium carbonate, $CaCO_3$) by heating it. This process happens in kilns, where raw material inputs (called 'raw meal') are heated to form clinker. Clinker is then ground with gypsum in a mill which becomes the end product, cement. There are two popular options to make clinker: dry and wet processes. The wet process receives a wet mixture of washed raw materials, which consumes more energy to dry the materials. We also model two grinding technologies: ball mill, which is more conventional, and vertical mill, which is more energy-efficient for a higher cost. CCS options for the clinker-making stage are added to the model, given the technical feasibility of the technology as well as the substantial emissions implications of this industry. Figure 4 shows the reference material system for cement.

Cement is usually only traded at low levels compared to other commodities, and the trade is usually used to balance out the surpluses and shortages across countries. Total cement trading accounts for 3-5% of total cement production volumes (Akram, 2013; Beirne & Kirchberger, 2021). As MESSAGEix-Materials operates in 12 world regions, cement trade is therefore not represented in the model.

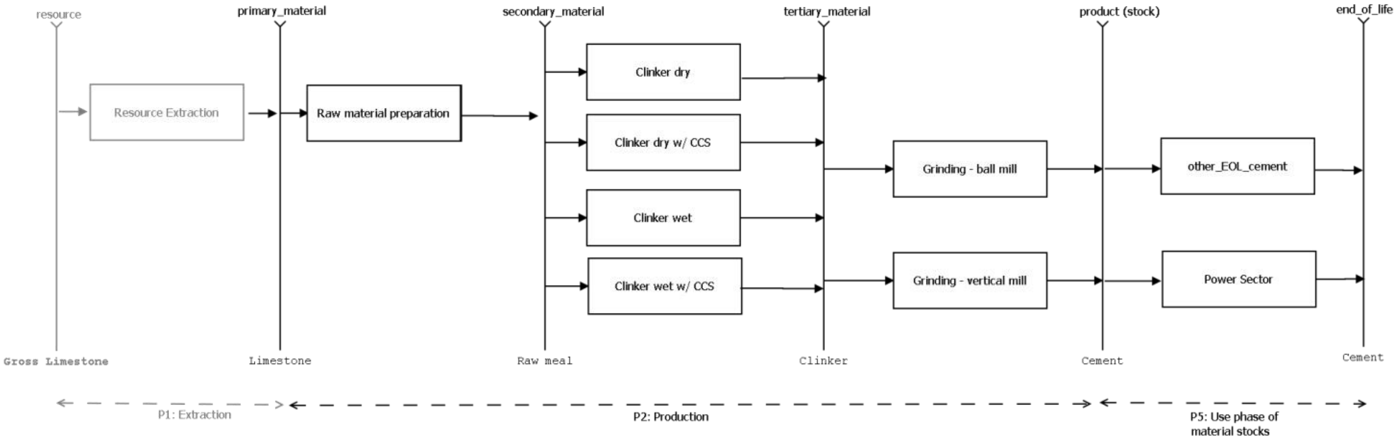

**Figure 4: Reference Material System for cement.**

### 2.2.4 Petrochemicals

The chemicals and petrochemicals industry accounts for 14% of total industry CO2 emissions, which amounted to 1.2 Gt CO2 in 2018 (IEA, 2020b). In 2020, final energy use, including feedstock use, reached 48 EJ, representing 30% of the industry's total final energy use (IEA, 2020a). Petrochemicals, a subset of chemicals derived from petroleum (oil) products such as naphtha or from natural gas such as ethane, are responsible for 90% of the total feedstock demand in chemical production in 2018 (IEA, 2018). Almost half of the energy inputs to the sector are for feedstock use which implies there are less CO2 emissions emitted from industrial processes compared to the steel and cement sectors and an important proportion of carbon remains in the final product.

Despite the complexity of the chemical sector, there are seven primary chemicals that provide the key inputs on which the bulk of the chemical industry is based. These primary chemicals are ammonia, methanol, ethylene, propylene and shortly known as BTX benzene, toluene, and mixed xylenes which account for approximately two-thirds of the sector’s total consumption of final energy products (IEA, 2018). In 2020, the production of these primary chemicals reached 543 Mt/yr (IEA, 2021a; IEA, 2018; Methanol Institute, 2022).

In the model, carbon contained in the chemicals and plastics products is represented under certain assumptions. To calculate an estimate of these carbon stocks, we differentiate products that are oxidized during use and long-lived non-oxidizing products drawing on the NEAT model which differentiates chemical products based on their chemical stability during use (Neelis et al., 2005). In addition, we make use of the ratios of primary chemicals that end up in plastics and the share of the plastics that go to incineration. 85% of the high-value chemicals and 65% of methanol are used in the production of plastics (Levi and Cullen, 2018). We use the plastic waste treatment projections of Geyer et al. (2017) to consider the CO2 emissions from waste incineration. According to these projections, 28% of the plastics are incinerated in the base year 2020 and the incineration percentage is assumed to increase to 50% in 2050 (Geyer et al., 2017). The carbon that does not end up in plastics (released due to oxidation during use such as solvents), the carbon released because of incineration, and the carbon lost in steam cracking are released in the atmosphere in the emission accounting. The rest of the carbon is treated as stored and not accounted for in the chemical sector emissions.

### High-Value Chemicals

The production of ethylene, propylene, and BTX, jointly referred to as high-value chemicals (HVCs) amounted to around 360 Mt in 2018 (IEA, 2018). HVCs are the main building blocks of plastics that are used in various end-uses ranging from packaging, and consumer goods to insulation in buildings. Refinery products are the most important feedstock to produce high-value chemicals. Therefore, the refinery representation is extended in the materials module to represent the intermediate products. Figure 5 shows the reference energy system for the extended refinery representation. Refineries can vary in terms of their structure and specific processes in different regions. In MESSAGEix-Materials, we represent a typical crude oil refinery reflecting the current operating refineries in North America based on PRELIM model (Abella et al., 2020). The processes that are represented include atmospheric and vacuum distillation, hydrotreating, catalytic cracking, catalytic reforming, coking, visbreaking and hydrocracking. The intermediate products of refinery are light and heavy fuel oil, naphtha, atmospheric and vacuum gasoil and residues, kerosene, diesel, gasoline, refinery gas and petroleum coke. These products can be used as feedstock in chemicals industry and the remaining is blended into two simple commodities light oil and fuel oil based on their densities. Products that are not explicitly represented in the refinery are lubricants, bitumen (it is part of vacuum residue but not a separate commodity) and paraffin waxes. *Pre_intermediate, desulfirized and intermediate* are levels added to represent the refinery products at their different stages.

Extension of the refinery enables detailed representation of the production of HVCs. Steam cracker is the main conventional technology that can use different feedstocks in different modes. The feedstock alternatives are two different types of gas oil (atmospheric and vacuum), naphtha, ethane, or propane. Each of these primary feedstocks results in a composition of HVCs with different ratios. Gas oils and naphtha are the products of the detailed refinery representation in the model while ethane and propane are formed by a natural gas processing plant. Production of ethylene from bioethanol is also included as one of the renewable production options. Bioethanol is supplied by ethanol synthesis via biomass gasification. The production pathways for HVCs are shown in Fig. 6. In addition, methanol-to-olefins (MTO) process is represented to produce high- value chemicals and explained more detailed below in methanol section. Trade is represented for high-value chemicals as a single commodity at the useful_material level.

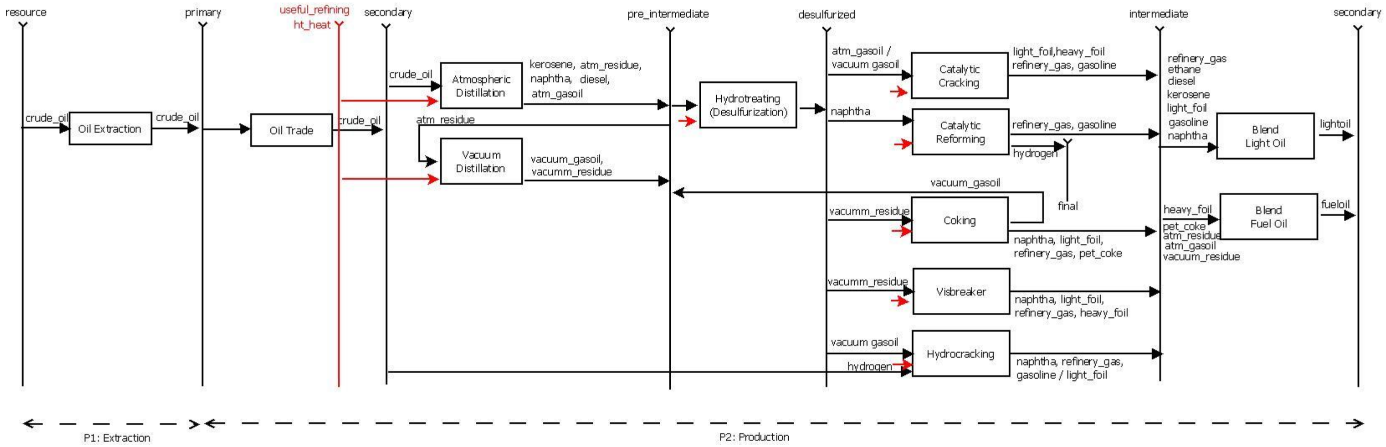

Figure 5: Reference Energy System for refinery.

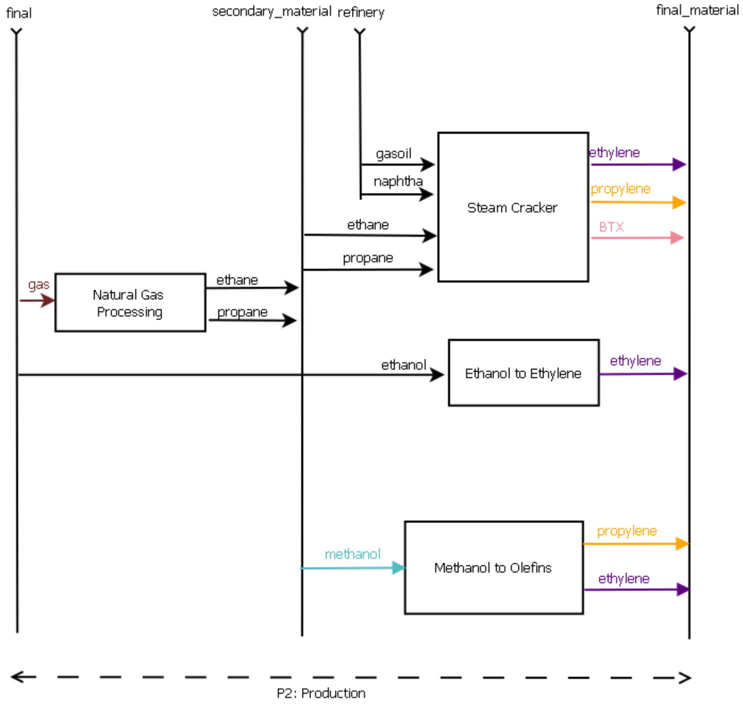

Figure 6: Reference Material System for high-value chemicals.

**Ammonia and Nitrogen Fertilizer**

Global ammonia production for both fertiliser and industrial applications was 185 Mt in 2020. In the same year, production was completely fossil based, 72% from natural gas, 26% was from coal and the remaining from oil (IEA, 2021a). Ammonia is input to all nitrogen fertilizer production processes. Among the nitrogen fertilizer products, urea-based fertilizer with high nitrogen content is widely used (58% of all N-based fertilizers in 2015) due to its high nutrient concentration and relatively low cost (Yara, 2018). Rest of the use cases for ammonia include cleaning products, refrigeration and air conditioning, production of plastics, textiles, explosives, food and beverage, and pharmaceutical industries. In addition, the use of ammonia as a fuel is promising as a carbon-free energy carrier produced via renewable sources and can be used in various applications, from power generation to transportation. However, there are remaining technical, safety and environmental challenges before it is adopted widespread.

MESSAGEix-Materials represents ammonia and N-fertilizer production processes currently with five different feedstock sources including coal, gas, biomass, fuel oil and hydrogen via electrolysis. In addition, we also model the low-carbon process of production with green hydrogen (also called “green ammonia”) and use of carbon capture and storage (CCS) technology for hydrocarbon feedstocks. As we are not interested in the material cycle of nitrogen, we do not represent specific types of N-fertilizers but treat them as a representative commodity type. For the trade implementation, currently MESSAGEix-Materials implements the trade of final N-fertilizer (about 30% of its production is traded) and the intermediate product ammonia (about 10% of global production is traded) (IEA, 2021a). In addition, GLOBIOM models the production, consumption, and the trade of the agricultural products. Figure 7 shows the reference material system for ammonia.

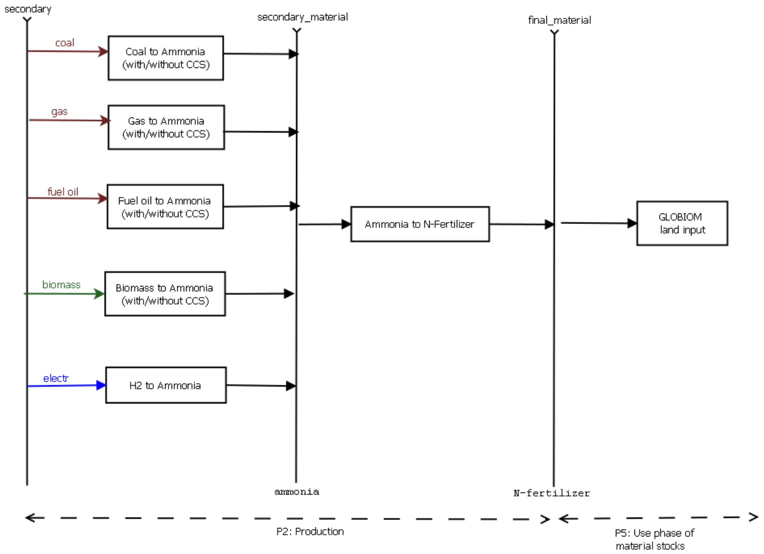

**Figure 7: Reference Material System for ammonia.**

### Methanol

Methanol is the third major base chemical of the petrochemical sector with just above 100 million tonnes of production in 2020 (Methanol Institute, 2022). Feedstock options are currently dominated by natural gas steam reforming and coal gasification. Coal gasification plants exist only in China but produce half of the total global methanol due to China's large methanol capacity. In MESSAGEix-Materials, various feedstock options are implemented including fossil (natural gas and coal) and low-carbon options with or without CCS. The low-carbon feedstocks are covered in the model with two technologies utilizing either biomass or syngas from hydrogen with captured carbon dioxide from CCS plants. In recent years, the production route "methanol-to-olefins" (MTO) has overtaken traditional chemical products as the single biggest methanol consumer. This technology is currently almost exclusively used in China but still consuming a considerable amount of methanol around 25% of total methanol production (Methanol Institute, 2022). Therefore, we include methanol-to-olefins technology in the model, which produces propylene and ethylene, featuring an alternative pathway to traditional oil-based petrochemistry. The second biggest share of methanol production is used to produce formaldehyde resins, which are mainly used in engineered wood products. The production of formaldehyde and the subsequent resin production is explicitly represented by individual technology instances to allow an endogenization of the methanol demand coming from the construction industry.

Besides traditional chemicals and MTO, a significant amount of total methanol production is used in various fuels. For an explicit representation in MESSAGEix-Materials, the production technologies can operate in "fuel" or "feedstock" mode. Figure 8 shows the reference material system for methanol.

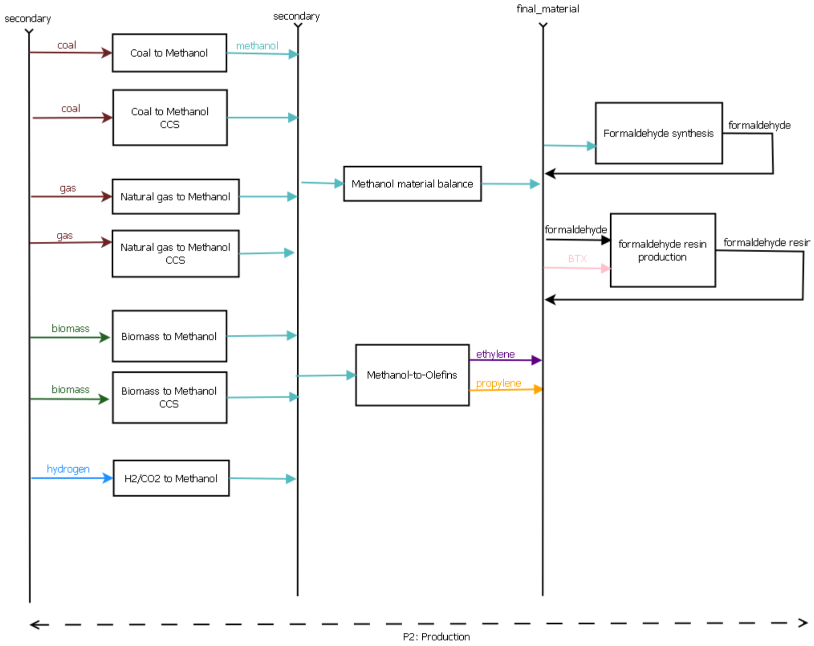

**Figure 8: Reference Material System for methanol.**

### 2.3 Material Demand

The demand for material stocks within MESSAGEix-Materials is determined in two different ways, depending on the end-use sectors. Section 2.3.1 explains the end-use sectors where material demand is endogenously generated, such as the power sector's material demand, the demand for nitrogen fertilizer, and some use cases of methanol. The process of deriving material demands from GDP projections exogenously is elaborated in Sect. 2.3.2.

### 2.3.1 Endogenous Material Demand

Electrification is an important element of the transformation to a low-carbon energy system and many low-carbon electricity generation technologies, in particular those based on renewable energy sources, have in general higher material demand per unit of installed capacity and in particular per unit of electricity generated than conventional thermal power plants (Arvesen et al., 2018). To incorporate this important linkage, we add material intensities for the most energy-intensive bulk materials used in power plant construction – steel, cement, and aluminium – to the MESSAGEix-Materials model. We rely on data from lifecycle analysis (LCA), specifically designed for the use within IAMs such as MESSAGEix-Materials (Arvesen et al., 2018). Upon construction of power plants, a demand for the three bulk materials is generated endogenously based on the material intensities in Arvesen et al (2018) per generation technology, vintage and region. Power sector material stocks exhibit specific lifetimes, and upon the retirement of the capacity, end-of-life waste material is released which then is collected and becomes available for recycling.

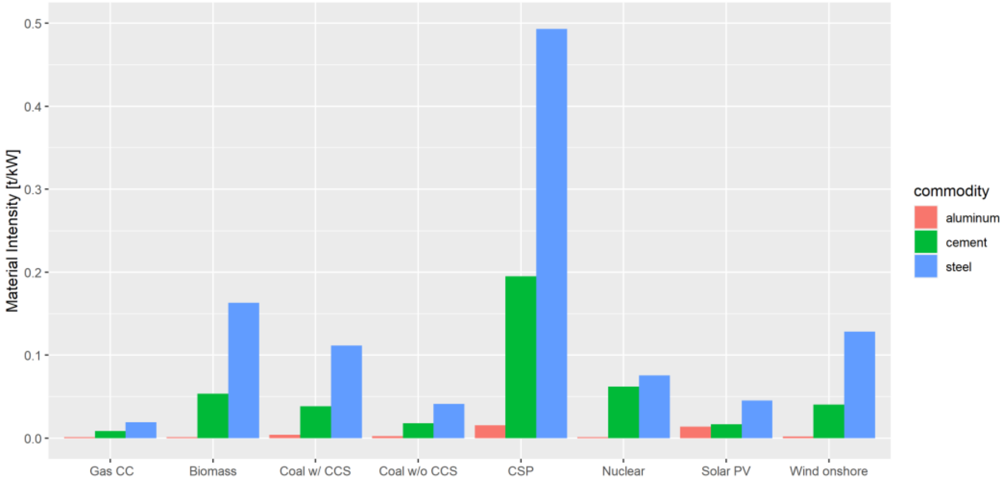

**Figure 9: Illustration of bulk material intensities for a subset of the electricity generation technologies in MESSAGEix-Materials. Data are shown for Western Europe in the year 2030. Source: 'mix' and 'residue' technology configurations from (Arvesen et al 2018).**

Figure 9 provides an overview of material intensities for an illustrative subset of the electricity generation technologies in MESSAGEix-Materials. As can be seen, low-carbon energy technologies tend to have larger material intensities than conventional generation technologies on average. However, two things should be noted in this context, (i) there is a significant spread with material intensities varying by an order of magnitude among the groups of low-carbon and conventional generation technologies, and (ii) material intensities per unit of installed capacity need to be put into context of total possible generation which is dependent on the operation time of the specific plant. These ratios (material intensity / total operation time), also vary considerably among the technologies with illustrative full load hours ranging from 1000 hours per year for onshore wind or solar PV under less favourable conditions to potentially more than 8000 hours per year at which many nuclear power plants are operated. MESSAGEix-Materials takes these factors into account when deciding for a cost-effective electricity generation mix under different climate targets.

The second end-use sector in which the material demand is endogenously represented is nitrogen-fertilizer demand. For the N-fertilizer demand projections, we use MESSAGEix-GLOBIOM emulator and import its synthetic fertilizer demand projections directly. Fertilizer demand in GLOBIOM is driven by future agricultural demand for food, feed, or other uses including bioenergy. The current implementation of the emulator includes next to a set of land-based climate mitigation scenarios also the representation of selected land-use related SDGs such as moving towards low-meat diets and halving food waste, that affect future nitrogen-fertilizer demand (Frank et al., 2021).

Finally, the methanol demand for the methanol-to-olefins route is linked to the high-value chemicals demand through the MTO technology. The methanol demand for fuel applications is driven by the oil product consumption of the transport sector and methanol can be also used as a fuel in industry based on the fuel choice of the model.

The material demand from the end-use sectors such as transportation and buildings can also be endogenized via linkages to the sectorial models such as MESSAGEix-Transport or MESSAGEix-Buildings which is planned in future work (Mastrucci et al., 2021).

### 2.3.2 Exogenous Material Demand

Total regional demands for three materials—steel, cement, and aluminium—are projected exogenously following the method suggested by van Ruijven et al (2016). This method chooses a best-fitting functional shape of the demand projection curve driven by per-capita GDP, which empirically is observed to have certain saturating behaviour for each country. With the data extended with more observational years, we estimate updated curves for the three materials. We have found similarly to van Ruijven et al (2016) that a globally non-linear model (NLI) with an S-shaped relation between GDP per capita and material consumption fits best for the cement and aluminium in Eq. (1) and a variant in which per capita material demand is reduced over time as a result of efficiency improvement (NLIT) in Eq. (2) fits best for steel. The global consumption curve is used as a starting point and individual curves are derived for major steel-producing regions. The global curve is calibrated to match the historical demand values for each region by modifying the maximum in the per capita consumption (PCC) curve (B) and per capita saturation level (a) parameters. In the formulation, T represents the time and C per capita consumption.

Non-linear inverse (NLI): $C = ae^{\left(\frac{B}{GDP}\right)}$ (1)

Non-linear inverse with time-efficiency factor (NLIT): $C = ae^{\left(\frac{B}{GDP}\right)} * (1-m)^{(T-2010)}$ (2)

Due to lack of comprehensive historical data for petrochemical demand, we derive income elasticities from IEA projections for high-value chemicals, methanol and ammonia. Subsequently, to project demand of petrochemicals the elasticities are used with the GDP projections from the “Middle-of-the-road” Shared Socio-economic Pathway (SSP2) (Dellink et al. 2017) that are adopted in MESSAGEix-GLOBOM. This approach is used to model the total HVC demand and residual demands for methanol and ammonia, which are not covered by the endogenous demand representation.

### 2.4 Modelling Approach

"MESSAGEix-GLOBIOM" refers to a family of global- and country-scoped IAMs developed in the MESSAGEix framework. This framework comprises the MESSAGE linear program (LP) and related tools. MESSAGE is a generic formulation of a least-cost optimization problem representing an abstract energy-economic-environmental system; it can (must) be parametrized to create models of any scope or resolution. The MESSAGEix-GLOBIOM model family parametrizes this generic LP with specific sets of technologies, spatial regions, time periods, and so forth. MESSAGEix is maintained and distributed as the open-source python package `message_ix`[2] with the core LP implemented in GAMS. This package also includes MACRO computable general equilibrium (CGE) model, which can optionally be parametrized and solved iteratively with MESSAGE as "MESSAGE-MACRO" to represent demand response to changing commodity prices. `message_ix_models`[3] is another open-source python package that provides tools to (a) build, (b) solve, and (c) post-process or ‘report’ solution data for models in this family.

MESSAGEix-Materials is published as a module within this `message_ix_models` package. Using this module, any base model in the MESSAGEix-GLOBIOM family can be augmented with additional structural detail related to industry sector, as described in Sect 2.2., and with data matching the resolution and parametrization of the base model. The MESSAGE LP is

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[2] https://docs.messageix.org/

[3] https://github.com/iiasa/message-ix-models
https://docs.messageix.org/projects/models/en/latest/

then solved with this added structure and data; and then additional post-processing routines derive quantities of interest from the granular, full-resolution solution data. Same modular approach is used to derive MESSAGEix-GLOBIOM variants with enhanced detail in the water-energy-land nexus (Awais et al., 2023), buildings, and transport domains.

Figure 10 demonstrates the modeling approach and the workflow. Relevant techno-economic data of industry technologies are collected from various literature sources that can be seen in Table S1 in supplementary and stored in either spreadsheet format or directly processed via python scripts. A MESSAGEix-GLOBIOM scenario is used as a base to build a scenario with the materials variant. One of the important advantages of this approach is that it enables easy integration with different MESSAGEix-GLOBIOM variants that have different spatial resolutions including country models (e.g., Orthofer et al., 2019) and different global region versions such as 11, 12 or 14 regions. The example scenarios presented in Sect.3 use the 12-region global model. The materials module consists of scripts to process and prepare the data for feeding into the model parameters. In the final stage, the model is solved together with all the equations of the MESSAGE-GLOBIOM model in an integrated way. The energy system consists of all the extraction and fuel conversion technologies from primary to the final energy level. The new industry sector technologies that are added from the materials module use energy from the final energy level as input to produce material outputs. The reporting code produces a reporting output that is used for analysis. In addition, the integration of MESSAGEix-Materials to the current MESSAGEix-GLOBIOM can be seen in more detail in Fig. S6 in supplementary material.

Representing the material flows for the power sector technologies requires changes in the model formulation, because version 3.7 of message_ix doesn't endogenously consider the flow of material commodities linked to installing and retiring energy technology capacities during construction and retirement in the "COMMIDITY_BALANCE" equation[4]. To endogenize material stocks and flows, the equation system of the MESSAGEix modeling framework had to be adjusted so that commodity flows are not only triggered by technology activities during the operational phase, but also by the construction, maintenance, and decommissioning of the technology capacity. This change in the equation system mostly affects the commodity balance equation and requires adding several parameters[5] for the material demand and release intensities. Further description of the modification of the equations and the newly added parameters can be found in Fig. S7 in supplementary.

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[4] https://docs.messageix.org/en/stable/model/MESSAGE/model_core.html#auxiliary-commodity-balance
[5] https://github.com/iiasa/message_ix/pull/451

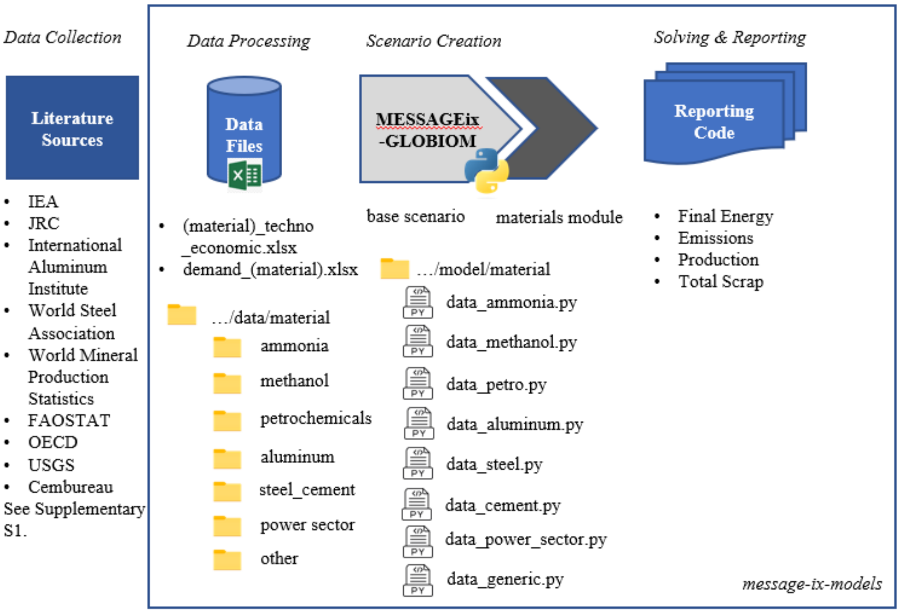

**Figure 10: Workflow for using the materials module.**

## 3 Model Results

### 3.1 Comparison of Base Year with Statistical Data

To validate the results, model values are compared with the reported statistics values in 2020 from different sources, mainly IEA. More specific information on the sources for this comparison is listed in Table S8.1 in supplementary. Final energy, CO2 emissions, and production values calculated with MESSAGEix-Materials are compared to statistics for the year 2020 as shown in Table 1. In the following, we discuss larger deviations that are beyond statistical uncertainties which are in the order of 10% for many quantities. For example, CO2 emissions from fossil fuel combustion and industrial processes according to the IPCC are known with an accuracy of about 8% (90% confidence interval; IPCC, 2023). In general, the variations in the comparison are due to the differences in the system boundary definitions. One industry that shows comparatively high variation is aluminium with 15% lower emissions in the model than in the statistics. This difference is attributed to the fact that the refining process which requires high-temperature heat (IAI, 2022) is not represented in the model. Iron and steel sector has 11% higher emissions compared to the statistics. Though this difference is still close to the 10% limit, the reason for observing a higher variation than the other sectors can be due to the reporting of the CO2 emission statistics with different system boundaries. Iron and steel is one of the industries where accounting for the final energy and emissions is more complex. MESSAGEix emissions and final energy values include the coke and coal inputs to blast furnaces, which is partly converted to blast furnace gas. The compared IEA final energy values include blast furnace and coke oven energy consumption but for the emissions, it is not clearly stated if these are also included in the reported direct CO2 intensity.

**Table 1: Comparison of MESSAGEix-Materials 2020 results with reported statistics.**

| | Aluminium | Steel | Chemicals | Cement |
|---|---|---|---|---|
| **Production (Mt/yr)** | | | | |
| (MESSAGE 2020, Statistics) | (100, 94) | (2038, 1880) | (505,543) | (4168, 4190) |
| Abs Diff | +6 | +158 | -38 | -22 |
| Rel Dif | +6% | +8% | -7% | -1% |
| **Final Energy (EJ/yr)** | | | | |
| (MESSAGE 2020, Statistics) | (5,5) | (34, 37) | (34, 37) | (15, 15) |
| Abs Diff | 0 | -3 | -3 | 0 |
| Rel Dif | 0 | -8% | -8% | 0 |
| **CO2 Emission (MtCO2/yr)** | | | | |
| (MESSAGE 2020, Statistics) | (169, 200) | (2971, 2670) | (928, 850) | (2635, 2435) |
| Abs Diff | -31 | 303 | +77 | +200 |
| Rel Diff | -15% | +11% | +9% | + 8% |

## 3.2 Comparison of Power Sector Material Stocks with the Literature

Figure 11 compares the estimates of the material stocks in global power plants for MESSAGEix-Materials with the studies from Deetman et al. (2021) and Kalt et al. (2021). Estimates of total power plant material stocks covering all generation technologies vary by a factor of up to seven due to differences in the material intensities and installed capacities. While the estimate of total stocks from MESSAGEix-Materials is within the range of literature sources for aluminium, it is slightly higher/lower for steel and cement respectively. Per technology, MESSAGEix-Materials stocks are within the range of literature sources for almost all technologies. An exception is hydropower, for which the MESSAGEix-Materials estimate is 9 times higher for aluminium and 5 times higher for steel than the highest value of other sources, and 37% lower than the lowest value of other sources for cement. The difference between estimates is partially driven by variations in assumed generation capacities by technology. Hydropower capacities in 2015, were assumed 13% lower than in other sources (Table S8.2 in supplementary), which can be a result of MESSAGEix model calibration to electricity generation instead of capacity. However, differences are primarily driven by variations in assumed material intensities for electricity generation technologies (Table S8.3 in supplementary). For hydropower, the material intensities assumed in MESSAGEix-Materials were 11 times those of the maximum of other sources for aluminium (6 times for steel), and only 76% of the minimum of other sources for cement. The difference in material intensities might be attributed to different types of hydropower having different material intensities (e.g., run-of-river vs. traditional hydroelectric dams with reservoir-storage). However, none of the sources distinguishes material intensities for these different types and instead uses one material intensity for all hydropower technologies.

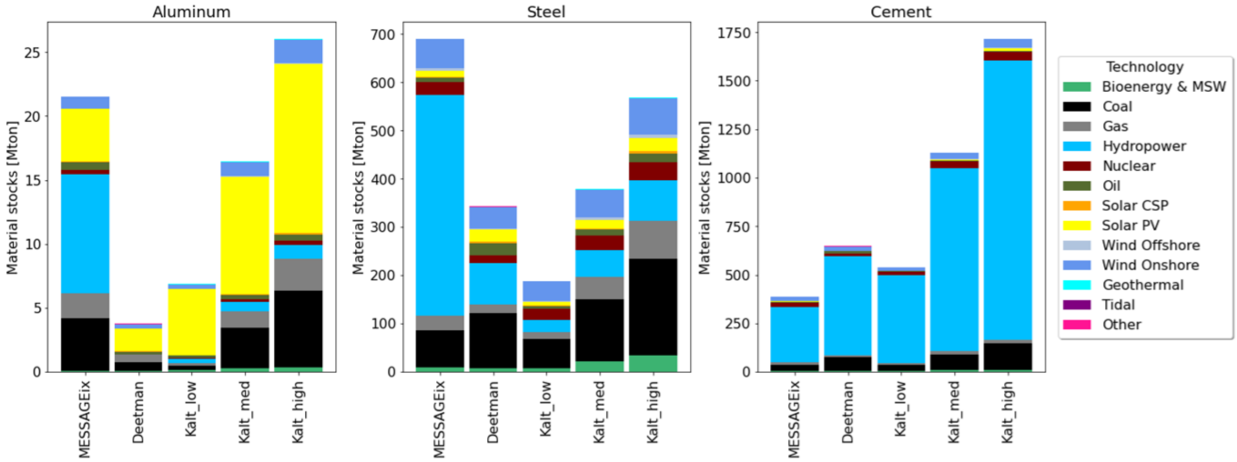

**Figure 11: Material stocks in global power generation technologies in 2015 based on this work (MESSAGEix-Materials), Deetman et al. (2021) and Kalt et al. (2021). The three estimates (low, med, high) by Kalt et al. (2021), result from using low, medium and high material intensity assumption as derived from literature. The technology categories in the figure slightly differ from those of MESSAGEix-Materials due to mapping of all three data sources to a common technology set. Similarly, the comparison shows cement instead of concrete stocks. To convert concrete to cement stocks for Deetman et al. (2021) and Kalt et al. (2021) results, a cement content of 15% in concrete was assumed. MSW = municipal solid waste, CSP = concentrated solar power, PV = photovoltaic. For figure data please see supplementary information S8.4.**

## 3.2 Scenario Comparison

### 3.2.1 Supply Side

The model results are compared for the two illustrative scenarios, 'NoPolicy' and '2 degrees' more specifically for the newly added industry sectors until the year 2070, the time at which total CO2 emissions roughly reach net-zero. 'NoPolicy' is a baseline scenario without any additional policy constraints beyond developments until 2020 and thus serves as a counterfactual whereas the 2 degrees scenario aims at limiting global warming to 2 degrees by the end of the century. 2 degrees scenario uses global uniform carbon prices from a "full century budget" scenario in line with 2 degrees (Riahi et al., 2021). A full century budget setup permits the budget to be temporarily overspent, as long as net-negative CO2 emissions bring back cumulative CO2 emissions to within the budget by 2100.

As opposed to having one single exogenous energy demand for the industry, including explicit material flows in the model produces more technology-detailed pathways for industry decarbonization with different insights for each represented industry sector. We find that, in the non-materials version of MESSAGEix-GLOBIOM there is slightly more reduction of industrial emissions than in those scenarios run with the explicit materials module (Fig. 12 & Table 2). In Fig. 12, until 2025, the estimates for 2 degrees scenario with materials module is stable, whereas without materials module emissions are already reducing. The limited potential for emissions reduction in the short term within the materials module may stem from the more restrictive growth constraints imposed to specific industry technologies. Subsequently, both the materials and non-materials versions exhibit a declining trend in the 2-degree scenario, with the non-materials version generally experiencing a faster decrease until 2055 as the specific reduction quantities are seen in Table 2. During this time NoPolicy scenario without materials module is growing faster which causes higher reduction of emission from NoPolicy to 2 degrees scenario in non-materials version as seen in Table 2. The primary factor behind this lies in the difference in the approach to representing demand between the two model versions, as detailed in Sect. 2.3. Finally, between 2060-2070, the emissions from the 2 degrees scenario with materials module is dropping much faster than without materials module. This can be attributed to the utilization of CCS technologies, particularly in the chemicals and cement industry, starting from this year onward, a feature absent in the non-materials version. Overall, MESSAGEix-Materials shows 45 Gt and 100 Gt higher cumulative CO2 emissions until 2070 compared to non-materials version in the NoPolicy and the 2 degrees scenarios, respectively. The first reason for this difference is the emissions gap in the year 2020 resulting from explicitly representing industrial production processes in materials module. In addition, this explicit representation also shows that the challenge of mitigating emissions from industry can vary at different times. As seen in this comparison, with the addition of materials module, mitigation is more challenging until 2060 and it is faster after 2060 due to CCS technologies. It's essential to interpret this insight while acknowledging that the model does not encompass each available option within the industrial sectors. For instance, it does not account for price inelasticity in material demands, and certain mitigation possibilities at the process level are not included in the analysis.

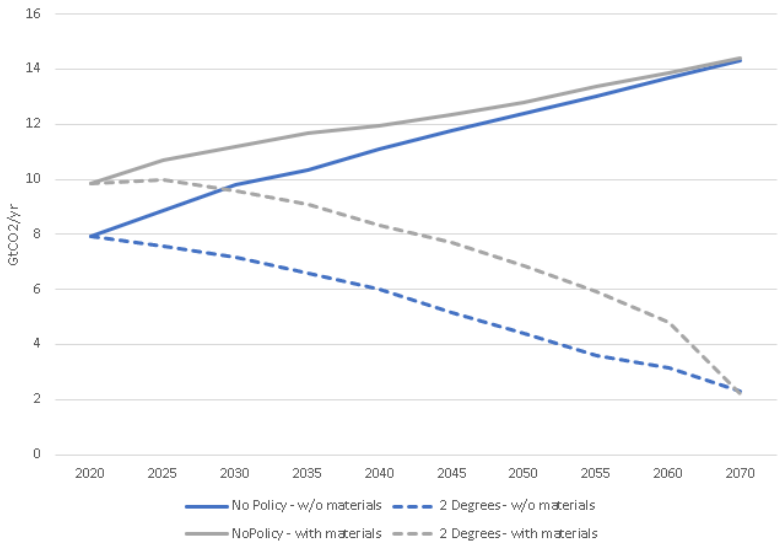

Figure 12: Comparison of industrial emissions with and without materials module.

**Table 2: Emission reduction percentages in 2 degrees scenarios with and without materials module.**

| Emission Reduction from NoPolicy to 2 degrees | 2020 | 2025 | 2030 | 2035 | 2040 | 2045 | 2050 | 2055 | 2060 | 2070 |
|---|---|---|---|---|---|---|---|---|---|---|
| Without Materials | 0% | 15% | 27% | 36% | 46% | 56% | 65% | 72% | 77% | 84% |
| With Materials | 0% | 7% | 14% | 22% | 30% | 38% | 46% | 56% | 65% | 85% |
| **Emission Reduction of 2 degrees from year t-1 to t** | **2020** | **2025** | **2030** | **2035** | **2040** | **2045** | **2050** | **2055** | **2060** | **2070** |
| Without Materials | - | 4% | 5% | 8% | 9% | 15% | 15% | 18% | 12% | 28% |
| With Materials | - | -1% | 4% | 5% | 9% | 8% | 11% | 14% | 19% | 54% |

Looking at the results from the materials module more in detail, we see that as a result of the climate policy, coal use in primary energy shows a substantial decrease in the 2 degrees scenario and instead is replaced by gas, wind, solar, and nuclear energy. Oil remains in the energy mix but to a lesser extent in the 2 degrees scenario. Looking at the CO2 emissions, in the year 2020, the industry sector has a 46% share of the emissions followed by the transport sector with 39% while the emissions from Residential, Commercial & Agriculture Forestry, and Fishery (RC & AFOFI) is responsible for the remaining 15%. In the year 2070 in the NoPolicy scenario, the shares remain almost the same for these end-use sectors. However, the 2 degrees scenario shows a substantial reduction of industrial emissions reducing its share of end-use emissions to 29% in 2070 while transportation rises to 63% indicating it is slower than the other end-use sectors to decarbonize. Primary Energy by fuel, Final Energy by end-use, and CO2 Emissions by end-use can be seen in Supplementary Fig. S9.1.

Figure 13 provides a more detailed look into the CO2 emissions and final energy from the industry sectors that are represented in the model and the remaining "other" that is not explicitly covered. Other industry includes industries such as equipment and machinery, food, beverages and tobacco, textiles and construction. In panel a, in the year 2070, despite its significant share in emissions, iron and steel is the sector contributing least to the decarbonization (2%) while a large chunk of the contribution comes from the other sector (50%). Chemicals is the next sector where high emission reduction is observed (36%). Cement follows this with an emission reduction share of 11% while the contribution of aluminium is minor (0.5%) as it has more indirect emissions coming from the production of the electricity rather than the production of aluminum.

Panel b and c of Fig. 13 shows the transition of fuels used in the industry sectors from a NoPolicy to a 2 degrees climate scenario. Final Energy Use excluding non-energy (b) most notably indicates a significant decrease in coal (37% to 7%) and an increase in gas (6% to 17%) and electricity (28% to 51%) shares from NoPolicy to 2 degrees in 2070. Hydrogen emerges as an alternative renewable source after 2050 from 0% to 8%, still with a limited share in 2070. The use of oil for high-temperature heat continues until 2040 in the aggregated other industry category in constant levels in both scenarios. Only after 2040, oil use starts decreasing in 2 degrees scenario. Similarly, for non-energy use (c) there is not much change between the NoPolicy and 2 degrees scenarios in terms of oil and ethane use. Their use as feedstock diminishes after 2040 in both scenarios and is replaced by coal in NoPolicy and by biomass in 2 degrees scenario. In both cases, this is due to biomass sourced methanol becoming one of the main feedstocks to produce high-value chemicals via the methanol-to-olefins (MTO) process. Panel d of Fig. 13 provides a more detailed look into the feedstock use in the production of high-value chemicals (HVC). The production routes do not change much between the scenarios but instead the source of methanol changes. In 2020, the feedstock of HVCs come from 27% ethane, 67% from oil, 4% from MTO and 2% from bioethanol. The bioethanol route does not scale up in the later years in 2 degrees scenario.

The regional dynamics of MTO (can be seen in Fig. S9.2) shows that in 2020, almost the entire 4% of the capacity is installed in China. However, this distribution changes in the future years, and after 2040 there is much more regional diversification. In 2070, we see that Former Soviet Union (FSU), North America (NAM), and Middle East and North Africa (MEA) are the regions that deploy more capacity than others. In addition, Latin America and the Caribbean (LAM) deploys more MTO in 2 degrees scenario switching to biomass as a source of methanol.

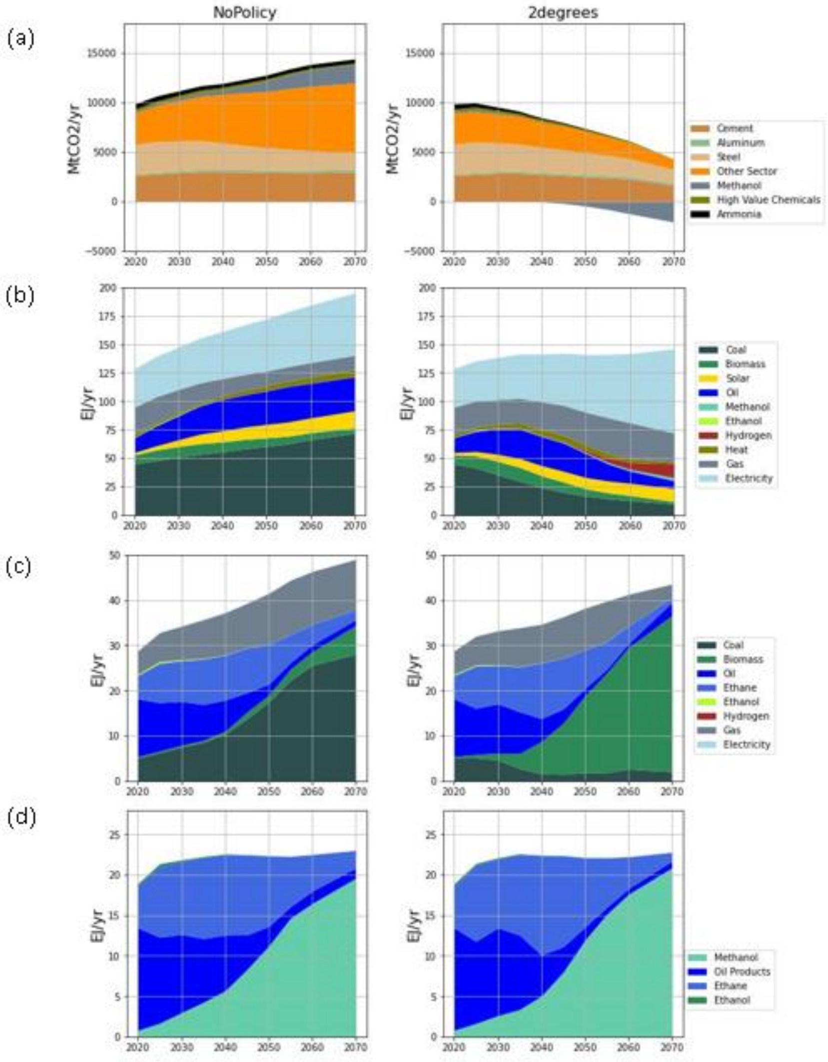

**Figure 13: CO2 Emissions and Final Energy for Industry (a) Direct CO2 Emissions by Industry Sectors (b) Final Energy Industry Excluding Non-Energy Use (c) Final Energy Non-Energy Use (d) High-Value Chemicals Feedstock Use.**

Final Energy use for the two other primary chemicals, ammonia and methanol can be seen in Fig. 14. Fossil fuel use continues in 2 degrees scenario for ammonia production however combined with CCS, capturing around 500 Mt CO2 in 2070 shown by the black line (panel a). For methanol production as mentioned earlier, the main feedstock switches from coal to biomass with CCS resulting in net negative emissions of more than 2 Gt CO2 in 2070 (panel b). Production via hydrogen is still not cost-effective compared to CCS and is not deployed for both chemicals in 2 degrees scenario.

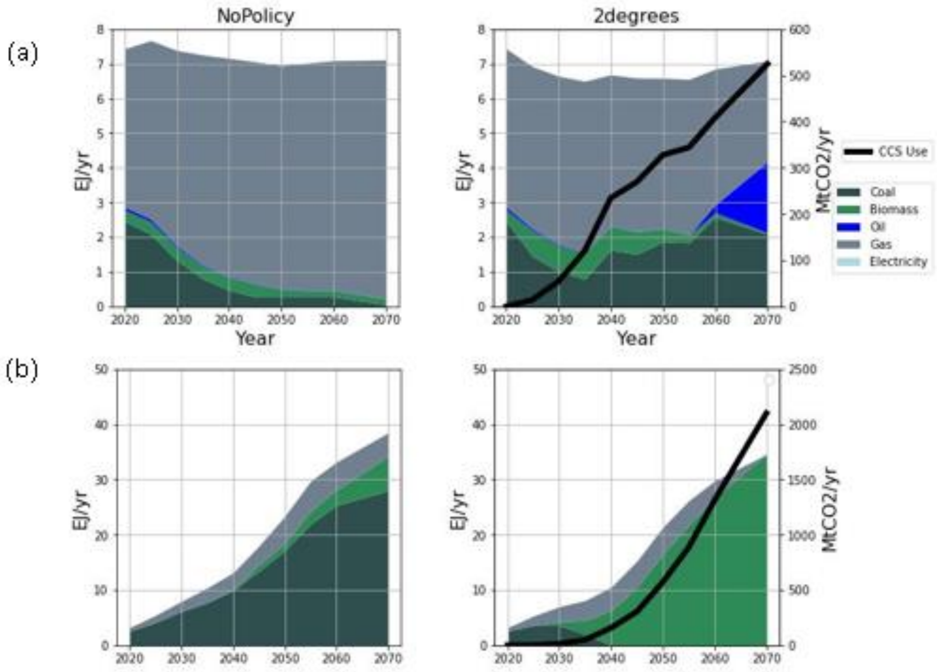

**Figure 14: Final Energy and CCS Use for (a) ammonia (b) methanol**.

Iron and steel as one of the major emissions-intensive industry has the lowest emissions reduction in the model with 2% of the total industry emission reductions in 2070. The technology mix of the iron and steel industry in Fig. 15 (a) shows that BF-BOF route that uses coal to produce primary steel keeps decreasing over the years from 69% in 2020 to 31% in 2070 in NoPolicy and to 28% in 2 degrees. Its share is replaced by the DRI-EAF and EAF-scrap routes. The levelized cost per unit production via the DRI-EAF route that use gas or electricity is lower compared to BF-BOF backed up by data, while the scalability and the replaceability between the two technology routes are not fully considered in the model. As the scrap availability increases over the years, EAF-scrap route with lower energy intensity also increases its share. The effect of climate policy is limited in pushing technological change in the absence of other decarbonization options such as the hydrogen production route or deployment of CCS in the model.

Figure 15 (b) shows the primary vs. secondary steel production (recycling) in NoPolicy and 2 degrees scenarios. In 2020, the share of recycled steel in crude steel production is 29%. In 2070 in both scenarios, the share of recycled steel in crude steel production rises to 48%. Differently, in 2 degrees scenario, climate policy enforces the use of scrap in the near-term until 2045 and therefore secondary production is 8% higher than NoPolicy between 2025 and 2040.

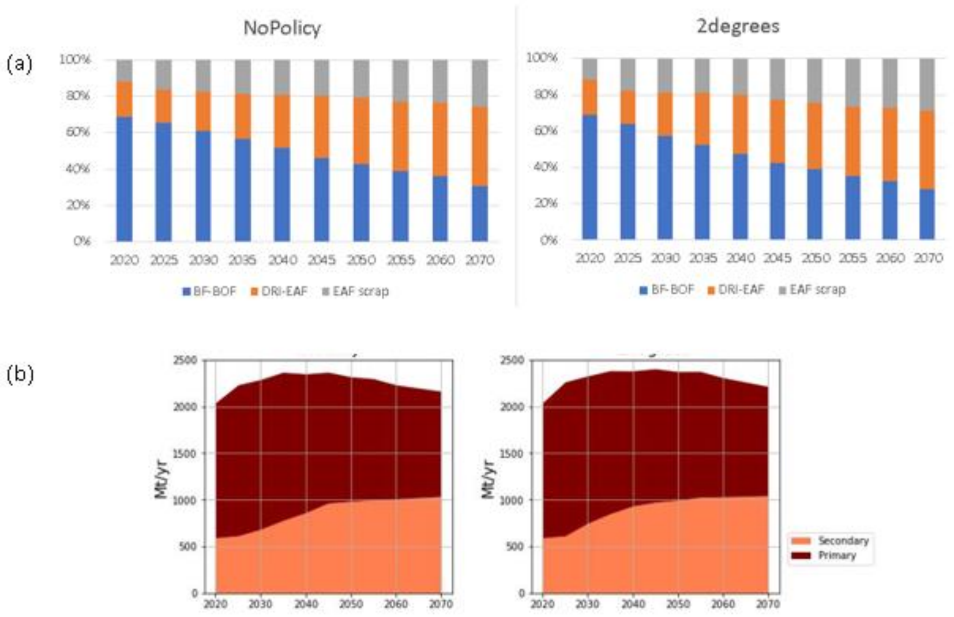

**Figure 15: Iron and steel industry (a) Technology mix (b) Primary and secondary production.**

Cement is another crucial industry that used coal to satisfy more than half of its energy needs in 2020. In the 2 degrees scenario coal use in cement production declines, and the use of gas and electricity increases until 2070 (Fig. 16). The electricity use increases particularly in the years 2060-2070 due to the rapid expansion of CCS. The black line in Fig. 16 shows the process-related CO2 emissions captured via CCS. The technology is only used after 2050 and captures 600 MtCO2 in 2070. To satisfy the high-temperature heat demand oil is still used in the 2 degrees scenario with a 6% share of the energy demand in 2070. Methanol is also used as another fuel source with a 16% share in 2070 as well as a limited amount of hydrogen with a 4 % share.

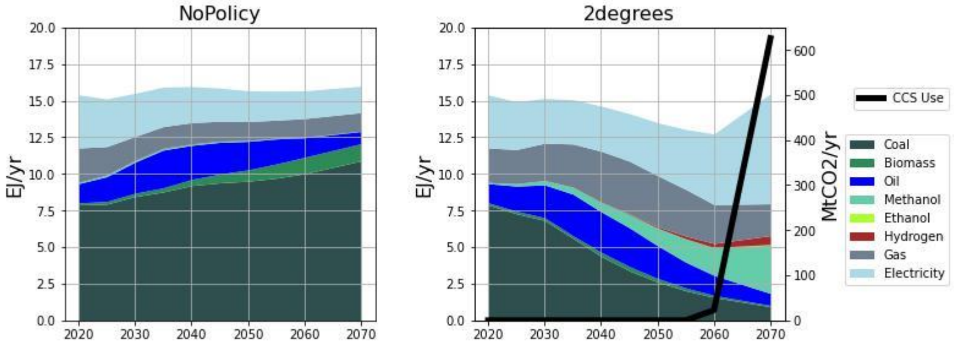

**Figure 16: Final Energy and CCS Use in cement industry.**

### 3.2.1 Demand Side

Currently, MESSAGEix-Materials derives the demand for materials either endogenously or exogenously as explained in Sect. 2.3. After an overview of the material supply side in the previous section, the following section provides results on material demand and stocks from the power sector as endogenously represented in MESSAGEix-Materials (see Sect. 2.3.1). Figure 17 shows the material stocks and technology capacities comparing the NoPolicy and 2 degrees scenarios. Because of the increased electrification, the overall capacity of electricity generation technologies increases in 2 degrees scenarios, specifically low-carbon technologies such as wind and solar. The overall increase in capacity naturally implies an increase in the stocks of three bulk materials aluminium, steel, and cement. In 2070, the 2 degrees scenario has 43% more electricity generation capacity than the NoPolicy scenario (23.6 TW in NoPolicy, 33.7 TW in 2 degrees). Accordingly, the total material needs of electricity generation technologies in 2 degrees scenario is 2 times higher than the NoPolicy scenario (2638 Mt in NoPolicy, 5327 Mt in 2 degrees). The share of increase in all three materials is close to each other.

Producing the extra 2700 Mt of the bulk materials to build the electricity generation capacity of 33.7 TW in 2070 is equivalent to a 1 Gt CO2 release considering the emissions intensity of the industrial sectors as in the 2 degrees scenario. The same increase in the material demand would be equivalent to 1.9 Gt CO2 emissions in 2070 with the emission intensities of the NoPolicy scenario. To put these emissions into a scale, one can compare them with the emissions reduction from the end-use sectors between the two scenarios. CO2 emissions from the demand side (transport, residential and commercial, industry) decrease by 21.4 Gt in 2070 in 2 degrees scenarios. Even though not all the decrease can be attributed to electrification, considering the increase from 35% to 51% in electrification on the demand side, we still can assume that the emission savings would be well enough to compensate for the increase resulting from the additional material demand. However, it should be noted that for a more complete picture of the material needs/stocks and for stock-flow consistency, all energy technologies should be considered including the replaced technologies by electrification (e.g., oil, coal-based heat providing technologies) which might increase the material demand in NoPolicy. In addition, transmission and distribution infrastructure is important to consider with the increased electrification which can increase the material demand further in 2 degrees scenario (Kalt et al.,2021; Deetman et al.,2021).

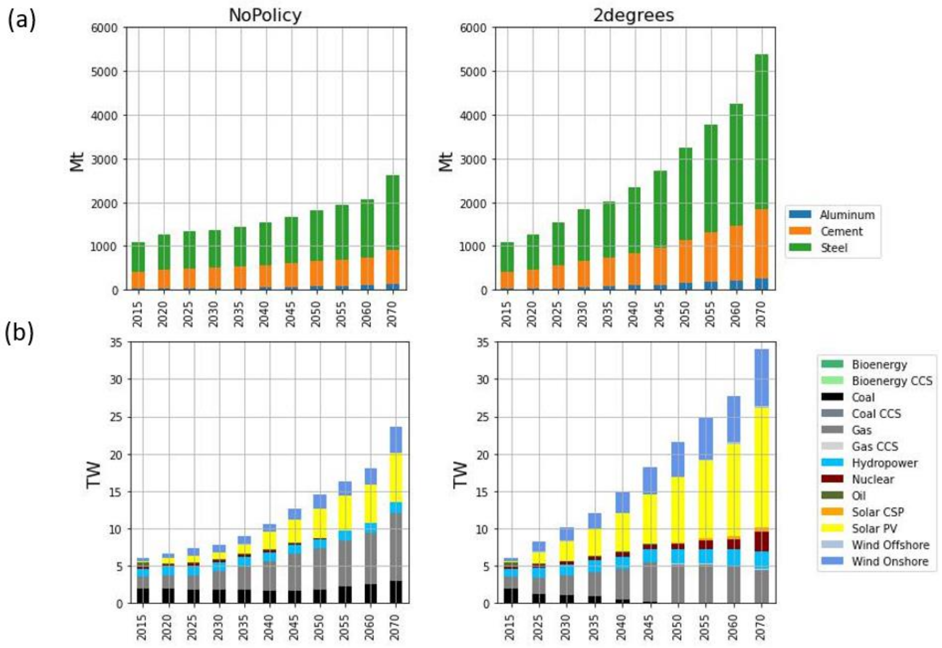

**Figure 17: (a) Power sector stocks by material (b) Electricity generation technology capacities.**

It is important to note that overall, in 2015, the material stocks of power plants are small, compared to total economy-wide material stocks. Per material group, power plant stocks make up for 1-2% (aluminium and steel vs. all metals) and 1-3% (concrete) of the economy-wide material stocks estimated by Krausmann et al. (2018).* Data on end-use of stock-building material flows suggest that the majority of these materials are used in construction of buildings, infrastructure and other machinery instead of power plants (Liu and Müller, 2013; Pauliuk et al., 2013; Cao et al., 2017). However, in addition to the material stocks in power plants, materials in electricity grids and storage technologies would increase the above shares, especially for metals. An exemplary investigation for electricity grids in North America with data from Kalt et al. (2021) and Deetman et al. (2021) showed that aluminium and steel in electricity grid infrastructure were 5-43 and 0.6-1.2 times larger than the material accumulated in power plants themselves (Streeck, 2022).

*the mentioned minimum and maximum shares here indicate the share of the respective minimum and maximum estimates per material over all three data sources shown in Fig. 11.

## 4 Discussion and Conclusion

The comparison between the NoPolicy and 2 degrees scenarios reveals that climate policy can have a major effect on industry sector emissions which are reduced by 85% in 2070. With the MESSAGEix-Materials module, we opened the partial blackbox of the industry in conventional MESSAGEix enabling us to identify where the mitigation potentials of different industry sectors come from. Iron and steel as one of the major emissions-intensive industry offers limited emission reductions from NoPolicy to 2 degrees scenario with 2% of industry emission reductions in 2070 just with DRI-EAF and scrap routes represented in the model as an alternative to BF-BOF route. Exploring additional decarbonization options such as CCS and hydrogen route in the iron and steel sector (not implemented here) would be important to evaluate further emissions reduction potential in this industry. The cement industry as the next major emitter, has 11% of the industry emission reductions from NoPolicy to 2 degrees scenario in 2070 mostly due to the CCS use to reduce the process emissions and to some degree due to switching to cleaner fuels such as electricity, methanol and hydrogen to provide high-temperature heat for the processes.

Chemical industry contributes to more than one-third of the emissions reduction from NoPolicy to 2 degrees scenario. Our scenarios show that oil, ethane, and gas remain to be used as feedstock in the chemical industry while scaling up the methanol-to-olefins (MTO) route offers a bio-based alternative feedstock to produce high-value chemicals. Even though today MTO route is mainly used in China with coal as a feedstock, in future years regional diversification could increase and biomass with CCS has the potential to be used as the main source of methanol production. CCS appears as a cost-competitive option both for ammonia and methanol over the years. Particularly process-wise CCS works well for ammonia production as ammonia requires hydrogen as a feedstock, typically made from processing natural gas or coal. A by-product of this process would be a high-concentration stream of CO2 meaning that the process is ready to allow capturing CO2. Some of the captured CO2 can be used to produce urea on-site with the remainder requiring compression and purification before it is ready to be transported or stored instead of going to the atmosphere. Around half of the emission reductions from NoPolicy to 2 degrees scenario originate from the "Other Industry" that is not represented at the process level in the model which includes energy-intensive industries such as paper and pulp or glass as well as low-energy-intensive industries such as food and beverages, mining, and textiles.

This simple scenario comparison exercise illustrates that the representation of the energy-materials nexus in integrated assessment models broadens the space of climate change mitigation options. We observe that incorporating explicit industry sector representation along with material stocks and flows can introduce both additional mitigation challenges and facilitate overcoming challenges, with effects varying across different time frames. By introducing additional industry sectors and mitigation options to the materials module, the impacts of mitigation challenges will become more evident in contrast to a version without material considerations. In addition, MESSAGEix-Materials facilitates sharing data within the modeling community and enables collaborative work on improving the data situation for techno-economic data in the industry sector by providing an open-source release of the model and the data.

Adding material-related dimensions into IAMs and subsequently utilizing them for circular economy-related analyses has its own challenges. IAMs primarily serve to examine the interplay between socioeconomics, climate, energy and land use systems in a quite aggregate manner. Conversely, industrial ecology tools, such as Material Flow Analysis (MFA) and Life Cycle Analysis (LCA), aim to trace and quantify material flows along with their environmental impacts and usually have more specific focus on certain products, sectors or materials. Consequently, it is challenging to bring together these two different scales. In addition, IAMs use a flow-oriented approach to e.g. represent energy commodities and therefore, representing stock dynamics and comprehensively addressing the entire life cycle, especially the aspects pertaining to end-of-life and recycling, poses a challenge since these elements are typically not relevant for conventional energy system representations. On the other hand, IAMs offer a set of distinct advantages over traditional industrial ecology tools. While industrial ecology tools by now have lots of material flows and stock data, the “techno-economic” layer such as costs, production capacities, lifetimes of capital stocks are not as detailed as they are in IAMs. IAMs incorporate techno-economics into decision-making processes, establishing feedback with the land-use system, and linking that to different energy carriers. In this regard, collecting the techno-economic data of material production technologies required by IAMs and the data on the regional differences for the technologies can be considered as another challenge to build up the materials module.

Version 1.0.0 of MESSAGEix-Materials serves as a proof-of-concept implementation for integrating material stocks and flows and holds potential for enhancement through collaborations between IAMs and industrial ecology tools. Creating a bridge between industrial ecology tools and IAMs is becoming more relevant to analyse the synergies between circular economy and climate mitigation options. In that sense representing the whole life cycle of the materials in the model will enable IAMs to integrate circular economy measures and their links to carbon stocks and flows more accurately. For example, one potential future work related to this includes extending the end-of-life chemicals sector representation by adding plastics production and recycling processes into the model.

Future work in particular regarding the supply side includes the further decomposition of the "other industry" aggregate in order to add further important energy-intensive industries such as paper and pulp or glass. By that, emission reductions resulting from changes in these industries can be uncovered. In addition, extending the supply side with materials that play a strategic role in decarbonization such as copper, lithium, nickel, graphite or cobalt is important for having a comprehensive coverage of materials. Looking at the materials demand side, the power sector represented in MESSAGEix-Materials, currently only requires a small share of the economy-wide material stocks. However, due to the increasing importance of electricity infrastructure and storage with progressing decarbonization of the energy and transport system, consideration of the material needs from electricity grids and storage technologies in MESSAGEix-Materials power stock estimates is a central future research agenda given the extensive energy system representation of IAMs. Future endogenization of economy-wide material demand and stocks could better represent the differences between the NoPolicy and 2 degrees scenarios in explicitly quantifying the additional material demand (and related energy use and emissions) not only for power generation technologies but also for grids, construction of buildings, infrastructure; transformations in the transport sector and related repercussions in industrial machinery. In line with this, endogenously connecting the material service demands (such as transportation or buildings) to the material production and end-of-life phase is crucial for better understanding the challenges of the transformation towards a sustainable low-carbon energy system (Mastrucci et al., 2021). This will also allow us to investigate the material, energy, and emission implications of securing decent living standards more consistently. GDP driven material demand does not consider biophysical limitations, but this shortcoming can be overcome by a consistent modelling of the stock-flow-service nexus that drives energy and material demand. With a broader set of materials covered and a larger fraction of demand becoming endogenous, there will be more climate change mitigation options to be explored in connection with circular economy. In sum, we expect this research area to continue to offer opportunities for further development and generate novel analysis and insights to complement more traditional mitigation options in the energy and land-use sectors.

## Authors Contributions

GÜ, FM, JM, VK conceived the modelling framework. GÜ, FM, JM worked on model development with the coordination and supervision of VK. JS provided analysis on the comparison of power sector stocks between the literature and MESSAGEix-Materials. SF provided updated land-use scenarios from GLOBIOM model. FG and PNK provided information and guidance on releasing the model as open source in message-ix-models repository. DW and NE contributed to conceptual framing and the development of the integrative system definition in relation to material flow analysis perspective. GÜ led the manuscript framing and writing, preparation of results and conclusions. All authors reviewed and contributed to the manuscript writing.

## Code and Data Availability

Version 1.0.0 of MESSAGEix-Materials is available on the website: https://github.com/iiasa/message-ix-models/tree/migrate-materials under the Apache License, version 2.0. The same model version (1.0.0) that is used to produce the results in this paper is archived on Zenodo (10.5281/zenodo.10370767), as are input data, scripts to run the model, and to generate the graphs for model results.

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## Competing Interests

The authors declare that they have no conflict of interest.

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