We sincerely thank the editor and all reviewers for their valuable feedback, which we have used to improve the quality of our manuscript. Here are our specific responses to the provided comments.

Responses to Referee 1:

To make improvements on these suggested points related to policy relevance of the paper and technology richness in different industries, we extended the representation of the iron and steel sector in the model. As suggested by reviewer, we include hydrogen DRI and CCS as well as use of biomass in blast furnaces in the new model version. We update the results and conclusions in the light of the newly added iron and steel technologies. As the main purpose of this paper is to serve as a methodological model documentation, we choose to use a NoPolicy and 2 degrees scenarios to validate the model but not a more elaborate scenario set with different climate policies and drivers. Scenarios with different policy aspects will be the scope of future papers. However, we included a few scenario variations in this paper to back up the results in the iron and steel and cement sectors. These are a net zero steel sector target scenario and a scenario with a very high carbon price that pushes the model to its limits to observe the uptake of the CCS technology in cement industry.

To address the comments about the timing of the CCS in cement industry, we have made some improvements in the model parametrization. These include cost revision for cement CCS and decrease of costs over time from 2030 to 2050 for cement CCS technology based on http://www.fp7-advance.eu/?q=content/industrial-sector-cement-guideline. The electricity and high temperature heat needs of cement CCS are also revised based on https://www.sciencedirect.com/science/article/pii/S0263876217303003) and https://www.sciencedirect.com/science/article/pii/S1876610209000150) as they were found to be on the higher end. In addition, a sensitivity run with an extremely high carbon price reveals the limits and upper bounds of the model in terms of the CCS deployment in cement industry. This is added to the supplementary material and to the results section. We conclude that the later uptake is a result of the techno-economic costs of the CCS technology in cement industry and the earlier uptake of CCS in chemicals industry aligns well with the technological readiness of the CCS in chemical industry. More explanation is added to the text on this issue.

It is mentioned that the mitigation potential appears similar to before the model improvements in 2070. This changes after the addition of the new iron and steel technologies and there is 94% reduction in industry related emissions in 2070, higher than the non-materials model version. Non-materials version has more reduced industry emissions in some years and more discussion is added on this as suggested by reviewer to Section 3.2.2.

Below are our responses to some additional points:

The rationale to choose to represent these materials is not clearly made explicit: The materials are primarily chosen based on their contribution to final energy and emissions in the industry sector. In addition, their end-use applications are considered for the potential to be combined with important demand side strategies such as the ones from mobility, built-environment, machinery or packaging in future papers. This information is now added to the beginning of Section 2.2.

Why choose to model aluminium instead of some other metal like copper?: Aluminum was chosen as one of the most energy intensive industries next to chemicals, iron and steel and

cement. Although the carbon footprint of primary aluminium varies largely depending on the source(s) of electricity used, the process is highly electro-intensive, requiring around 14 MWh per tonne of metal, about seven times more than copper smelting. Aluminium production requires around 40% more energy than copper ((CRU copper: https://www.crugroup.com/knowledge-and-insights/insights/2021/cru-explains-copperaluminium-smelting-emissions/).). Copper is being included in another version of the model not due to energy and emission intensiveness but for concerns of availability in the case of increased EVs in mobility.

The choice to explicitly model materials flows related to power generation technologies needs to be justified more: Currently, the power sector does not constitute a significant share of the materials used. Despite that, the first reason for examining this sector is to determine how much this situation changes under climate policy, where the demand for power generation increases. This can also be complemented with the material needs of transmission and storage. The second reason is more operational: power sector technologies are already integrated into MESSAGEix as part of the energy systems model and therefore is a good starting point for testing the initial implementation of the changed model formulation. This change in the formulation that allows considering the flow of material commodities linked to installing and retiring technology capacities can also be used to represent other stocks endogenously. Incorporating other sectors, like buildings, require extra structural additions to the model. This type of study is planned but for a paper that focuses more on scenario and policy analysis whereas for the initial implementation we prefer to use power sector as a test case. An explanation is added to Section 2.3.1 Endogenous Material Demand.

Link to the code and data. The manuscript does not present several of its quantitative assumptions (especially regarding techno-economic parameters for production processes): The link to the GitHub repository that includes the code is provided in Code and Data Availability Section. The data sources for techno-economic parameters are presented in Supplementary 1. The data itself is not presented directly in the text as there are many technologies in the model with various parameters and it is difficult to fit all the data in the text. However, the model data is accessible in the open-source model version in excel format separately for each industry including all the inputs and costs. The specific link for this is also provided under the Code and Data Availability Section.

Below are our responses to more detailed comments:

Line numbers based on the initial version of manuscript as used by the reviewer.

L168-172: The description first describes what is implemented in the model for each phase P1, P2 etc. Then discusses what is not yet included in the current version of the model but are expected to be extended in the later model version by using a similar approach to the current representation. Extraction is modeled for the feedstock materials such as coal, oil, gas which are used in chemicals industry. The trade of these material is also represented in the model. For the other raw materials which are not as much as detailed as the chemical's feedstock, there is an exogenous average raw material price attached based on the current market for the base year. The price is discounted into the future with a rate of 5%.

L186 it's not clear how the scrap levels 1/2/3 are determined: Scrap level 1/2/3 are qualities of scrap which also affects the ease of scrap preparation. Level 1 has the highest quality (e.g., least impurities, least copper contamination) therefore it is less costly and energy intensive to

prepare this type of scrap before the recycling step whereas 3 is the lowest quality. This type of scrap requires more technologically advanced sorting and dilution methods to be able to be used as recycled metal in any application. We can connect this information with the reference material system diagram as follows: At the moment in the model power sector and other endof-life products release scrap and this is accumulated in total end of life1/2/3. It is assumed medium quality scrap (level 2) has the highest availability with 50% of total scrap and the rest of the availability is divided between highest and lowest quality scrap (1 and 3). After this the scrap is recovered from these levels if the model prefers to use it based on production costs. The different energy and costs are associated with the scrap preparation 1 2 3. This version of the model can be used as basis to associate the different scrap quality levels with end-use sector demands if model is connected to other end-use demands such as vehicles or buildings. For example, end-of-life vehicles, machinery parts followed by electronics are the highest copper contaminating old scrap sectors, while the new cars are the main end-use behind the demand for higher (https://pubs.acs.org/doi/10.1021/acs.est.7b00997, the quality steel. https://www.sciencedirect.com/topics/materials-science/copper-scrap). However, this is not done in this version. More clarification is added to the text on these points.

L212, L232: Changed as suggested.

L271: Changed to World Steel Association.

L296: Drivers and cost components that are included for trade: A more detailed explanation about this is added. Cost components considered are shipping costs as in the form of variable costs and the cost related to building an export capacity which includes the necessary infrastructure and logistics resources. The drivers of the trade are the production and trade costs which are driven by different factors such as existing production capacity, fuel prices and historical trade activity. More detailed explanation is added to the text.

L314: Energy demand for refining: Refining step for aluminum is added to the model to extend the coverage.

L318: Why were two aluminum technologies singled out: These two technologies are the ones that are used commercially at the moment for aluminum production therefore they are included in the model. The difference between two technologies is added to the text.

L339, L341: Clarified as suggested.

L364: The model includes the chemicals demand and production processes for the primary chemicals: ammonia, methanol, ethylene, propylene and shortly known as BTX benzene, toluene, and mixed xylenes. Since BTX is also included in the model it is mentioned in the introduction here. The sum of ethylene, propylene and BTX are referred as high value chemicals in the rest of the paper. In the text, a clarification is added for classifying BTX under high value chemicals.

L371: Source and data for these rations and shares: The source is (Levi and Cullen, 2018) mentioned at the end of the sentence.

L399: Changed as suggested.

L417: More detail on how ammonia-as-a-fuel demand is calculated in the model: This information is provided in Section 2.3.2 Exogenous Material Demand. The approach is the same as deriving the petrochemicals demand.

L423: The sentence is changed.

L446: Clarified as suggested.

L448: More details added as suggested.

L485: Clarified as suggested.

L495: Beginning of section 2.3 explains some demands are exogenous and some are endogenous. Additions are made to clarify it better in Section 2.3 and 2.3.1.

L503: Discussion on the methodological choices to calculate materials demand: Some more explanation about the justification of aggregate GDP method to project demand is added to Section 2.3.2. The advantages and disadvantages of endogenizing material demand vs using the aggregate GDP based demand are discussed more in the Discussion and Conclusion Section. Here we also mention the future work on endogenously covering material demands for example for buildings and vehicles.

Regarding the question about total vs net material demand: The material demand for aluminum, steel and cement are derived for the total of the material demand. The demand is exogenously projected for the total of HVC demand and only for the residual demands for methanol and ammonia, which are not covered by the endogenous representation as mentioned in Section 2.3.2.

L516: Method to derive chemicals demand: Unlike aluminum and steel, it is difficult to find a comprehensive historical data for chemicals therefore we had to opt for an alternative method to project the chemicals demand. The text is modified to describe the methodology that IEA uses. However, the source data that IEA use is not publicly available. Therefore, we use implicit income elasticities derived from their projections.

L559: Other flows for operation, maintenance, and decommissioning: Material intensities in Figure 9 are used during construction phase and released at the end-of-life. Decommissioning is also mentioned in the explanation of Figure 9 with these sentences: "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". The operation and maintenance flows are not included in this model version. To clarify, this information is added to the explanation section of Figure 9.

L567+: Explanation related to the differences in production, final energy and CO2 emissions are added. Also the values are updated with the new model runs and updated statistics. The changes are:

- Aluminum, steel, chemical, cement production values are updated from the most recent model run.
- Aluminum statistics source changed to International Aluminum Institute 2020 global aluminum cycle.
- Steel production statistics changed to World Steel Association.
- Alumina refining stage added to the model. Therefore, the final energy and emissions value for aluminum are updated to the recent model run.
- Final Energy statistics value previously excluded the refining part for aluminum. It is updated to a value that includes refining as well.
- Final Energy and CO2 Emissions values for steel are updated to the most recent model run after the addition of new iron and steel technologies. In addition, the final energy value from the model for steel does not include the cokeoven inputs.
- The source of statistics for Final Energy steel is changed to IEA Energy Balances directly. From energy balances, what is reported under iron and steel and blast furnaces are summed and cokeoven sector is excluded.
- CO2 emissions statistics value for steel updated based on the new production value from World Steel Organization.
- CO2 Emissions for chemicals are updated to the value from the most recent model run.

L597: High value for hydro: Arversen et al., 2018 provides three different material intensities for the hydropower plant. "1" is a hydropower plant with reservoir in a remote location, "2" is a hydropower plant with reservoir in nearer location and "mix" is both types considered by using market shares of these types. In our model we represent both run-of-river and reservoir types but not exceptional cases such as reservoirs that are in remote locations. Therefore, we choose to use Kalt et al., 2021 medium value for hydropower to be closer to the literature average and as it better fits to the types of hydropower we represent in our model.

The reference for Deetman is included in the list of references:

Deetman, S., Boer, H. S. de, van Engelenburg, M., van der Voet, E., and van Vuuren, D. P.: Projected material requirements for the global electricity infrastructure – generation, transmission, and storage, Resources, Conservation and Recycling, 164, 105200, DOI: 10.1016/j.resconrec.2020.105200, 2021.

L615: 2 degrees scenario can reach net-zero and go below to net-negative emissions globally to bring back cumulative CO2 emissions to within the budget by 2100. But there is not a net-zero constraint to force the model. Instead, a carbon budget assumption of 1000 GtCO2 is implemented. This is also added to the text. As a result of the implemented budget, model reaches net zero between 2070 - 2080 and has negative emissions in 2080.

L627: Changed as suggested.

L637 & Figure 12: We have done some further calibration of 2020 industry emissions in the new model version and now it is closer to the 9000 which reported by EDGAR6 and CEDS data sources. Also, the model version without materials is updated to a more recent calibration. This reduced the emission difference between two models. Both materials and non-materials version cover the whole industry. There is still a small amount of difference remaining between the two models as the calibration methods used are different for these two model versions as a result of the structural differences that comes with the materials module. However, this difference is within the uncertainty limits (5%) of the reported industrial emissions. The comparison related to cumulative emissions is removed and the explanation in the section is updated.

L642: It should have been price elasticity. Changed.

L651: Changed as suggested.

L661: More discussion is added as suggested.

L666: Added as suggested.

L669: This section is to get an overview of the total industry final energy. Graphs for specific industry sectors are provided and discussed more in detail in the rest of the results section. In addition, panel c non-energy use does not have any other sector but completely the newly added model results. To provide more information on the other sector final energy, a graph is added to the supplementary material.

L679: Added as suggested.

L708: Those technologies are added to the new model version as suggested.

L713: In No Policy scenario not all the scrap is used as not all regions have the electric arc furnace capacity and it is not economic to install these from zero just to use the scrap. However, in 2 degrees scenario, there is an increased adoption of electric arc furnaces motivated by reducing the emissions and as a result more scrap is used. The total scrap availability between two scenarios do not change except the minor effect of power sector scrap that is endogenously released that can be different in scenarios. This information is added to the text as well.

L722: Late CCS in cement industry: This question is answered in the first section of the response and more information is added to the cement results section.

L726: The increase comes both from electric kiln and CCS electricity requirements. This is added to the text.

L729: The order is changed as suggested.

L802, L825: Removed as suggested.

L845: Biophysical limitation mentioned here refers to the improvements envsiaged to cover a broader range of material stocks and flows that can reflect material demand better instead of GDP based projections. Material flows directly linked to service demand (e.g., passenger kilometer mobility demand) will offer a more accurate estimation of resource needs, while accounting for stocks based on their lifetime will improve the estimation of end-of-life flows and the availability of recyclable materials. The sentence is rephrased.

Responses to Referee 2:

In various parts of the manuscript, with the revised version we try to make it clearer to the reader what is included in the model and what is not yet included. Information on the methodological advance, its purpose and potential future uses is distributed over introduction and discussion and conclusion sections. We improve the discussion and conclusion section to

provide some more concrete examples on the future uses and to emphasize the methodological advance and its purposes.

Regarding the comments about Figure 1, material demand is not completely endogenized yet, but this is the ultimate goal. To clarify this in the figure (that not all of material demand is exogenous), we change the label as "Rest of the material demand". Energy demand in the figure refers to the useful energy demand which is exogenous in MESSAGE (<u>https://docs.messageix.org/projects/global/en/latest/energy/demand.html</u>). Fuels used to satisfy the useful demand and therefore final energy is determined in the model. Energy demand in the figure is the useful energy that is provided exogenously for the "other industry", residential and commercial and transport sectors. The label is changed as Rest of Useful Energy demand. The dashed area is the system boundary of MESSAGEix-Materials and outside of the dashed area is not covered endogenously in the model which is shown in the figure legend. Some clarifications are added to the text about what is included and what is not.

As suggested, more details are added on how trade is modeled, calibrated and what type of costs are considered. Also, information is added on how supply regions and potentials are determined.

We add more justification about line 348 for the lack of trade representation in the model for cement.

A comparison of results for iron&steel and cement industries with the similar studies is added such as: van Sluisveld et al. 2021, Muller et al. 2024 and Keremidas 2024.

More details are added related to circular economy and decent living standards applications and the benefits that the new model advancements bring. In addition, the discussion and conclusion section is divided into 3 sections for a better structuring.

Responses to minor comments:

Line numbers based on the initial version of manuscript as used by the reviewer.

- L39: Removed the word optimization.
- L193: The parameterisation and formulation used for recycling is added to the supplementary information.
- L313: The term "significant is removed and absolute values are added.
- For the figures that include more information such as aluminum and steel, or generic reference material system, the figures are converted to landscape format.
- L825: An article before "circular economy" is added.