Assessing critical materials demand in global energy transition scenarios based on the Dynamic Extraction and Recycling Input-Output framework (DYNERIO)

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Abstract

The energy transition process calls for striving interventions at global level towards the switch to low-carbon and green technologies. Such technologies surely impact positively in the direction of reducing the greenhouse gases emissions; however, their massive deployment brings along intense raw materials exploitation. Some of these materials have already been classified as critical due to their scarce availability: their crucial geopolitical role is then becoming more and more relevant, resulting in several attempts of quantifying the materials impact of energy transition scenarios.

While the majority of the analysed studies adopts purely LCA-based methodologies, this article presents a novel hybrid approach to assess the impact of transition pathways on raw material extraction, which includes both LCA-based and energy modelling features. Such approach has been formalized in a modelling framework named Dynamic Extraction and Recycling Input-Output framework (DYNERIO) and it has been integrated in the open-source platform for input-output analyses handling, MARIO (Multi-functional Analysis of Regions through Input-Output), which the authors contributed to develop. DYNERIO is composed by two soft-linked modules: the first module is an environmentally-extended Multi-Regional Input-Output (MRIO) model, which allows for economic and environmental shock modelling and impact assessment; the second module consists of a linear programming optimization energy model, dedicated to the assessment of regional extraction and recycling of critical materials based on the results of the MRIO model.

Beside the standard environmental and economic impact indicators, such as GDP and CO2 emissions, DYNERIO returns the yearly operating and disposed capacities for energy technologies required to meet the production of exogenously defined final energy services, and the consequent raw materials extraction and recycling. A simplified case study, based on the Exiobase hybrid-units database (version 3.3.18), is then proposed to demonstrate the framework capabilities. In such case-study, a simplified energy transition strategy is analysed, by implementing a set of announced policies as a technological perturbation in the MRIO module and evaluating their implications in terms of raw material dependence.

Keywords

Raw materials; energy transition; recycling; input-output analysis; impact analysis; DYNERIO.

1. Introduction

During the past decades, the worldwide scientific community approached more and more the concepts of sustainable development and transition for a low-carbon future. The widespread growing concern about the global climate challenge calls for striving interventions, nonetheless, whilst the low-carbon transition would foster the achievement of environmental goals, it requires large technology investments and deep changes in behavioural dynamics to be effective. Such efforts have not been put in place with the same emphasis among the endorser countries [1] and potential criticalities related to energy infrastructure [2] and on economic growth [3] may be encountered if massive measures are taken to keep faith with the Paris Agreement.

Moreover, together with the climate commitment, many other pledges concur along the pathways to sustainability, as stated from the UN Agenda 2030 [4], and energy is a cross-cutting topic among them [5]; therefore, a broader perspective when dealing with modelling the energy transition is required. One of the key issues on the board when dealing with sustainable energy transition modelling are raw materials. In the last decades, the consumption of raw materials raised significantly, driven by industrialisation and population growth [6] and, according to the latest IEA report on the topic [7], the extraction of such materials would most certainly represent the crucial bottleneck on the path to deep decarbonisation.

Energy transition is a complex process, encompassing not only technologic but also economic and social dimensions. Low-carbon solutions, such as renewable energy technologies and electric vehicles, are forecasted to be adopted massively to meet emissions reduction goals. However, their embedded content of critical materials leaves open discussion on geopolitical and energy security problems in the future [8]. Assessing critical materials demand within a global scope while massively deploying renewable and green technologies is therefore crucial to address a comprehensive scenario analysis on energy transition. Energy scenarios for future sustainability shall be, therefore, projected not only to capture how energy conversion systems could be designed to achieve selected goals, but also to define which are the implications of such systems on their supply chains.

To deal with the mentioned challenges, modelling energy transition calls for integrated frameworks [9], traditional bottom-up technology rich energy modelling frameworks, generally adopted to define least-cost technically feasible pathways, are linked and interact with a variety of Industrial-Ecology based approaches [10], correcting feasible pathways and enriching the related narratives.

1.1. Quantitative critical materials assessment: a review

The results of a literature review on critical materials assessment characterized by a macroscopic global perspective are here provided. Specifically, the review is based on the research of papers published after year 2010 in peer-reviewed scientific articles listed in the Scopus database, identified based on the following keywords: “energy transition”, “critical materials” and “scenarios”. At the date of the research, the database returned 56 article documents, among which the most cited and relevant 35 have been selected and taxonomized in Table 1 based on the following criteria: research focus, methodology, space and time scopes.

Regarding the research focus, the vast majority of the analysed studies concentrates on the assessment of critical raw materials requirements in future scenarios, often considering the impact of recycling and circular economy practices. The main difference among such studies regards the underlying methodology they adopt to perform their analyses. A first category of studies make use of data- or ad-hoc indicators-based methodologies. Rollat et al. analysed industrial consumption trends to assess the availability of rare earths elements (REE) in Europe [11]. Månberger and Stenqvist estimated how a 2060-oriented global decarbonization scenario would impact on the demand of 12 metals by adopting IEA and other literature data related to power and transport technologies [12]. Similarly, Beylot et al. investigate the requirements of steel, aluminum, copper and concrete according to scenarios assumption based on climate-related target set by the French government by 2050 [13], while Kiemel et al. estimated the future materials bottlenecks to be supplied for the electrolyzers production in Germany up to 2050 [14] and Sun et al. analysed the risks for future supply of critical metallic resources useful for the global production of lithium-ion batteries [15]. An interesting work from Zhou et al. dealt with the issue of rare earths being by-products of other materials while estimating, via the calculation of suitable indicators, the demand of such materials for the supply of PV technology at global scale up to 2050 [16].

On the other hand, other articles performs materials requirements forecast analyses with more structured frameworks and methodologies, improving the replicability of the study but limiting its depth and focus. The most diffused methodology is surely the dynamic material flow analysis (dMFA), also frequently adopted within the sample of studies selected in the literature research performed. dMFA is a consolidated industrial ecology methodology allowing for accounting flows and stocks of available materials along supply chains. Among many noticeable applications, Elshkaki and Shen assessed the global implications of the use of critical metals in China with a time horizon at 2050 analyzing seven reference energy scenarios [17]. Similarly, Ren et al. evaluated the impact of photovoltaic penetration in China, focusing on the metal bottlenecks. Cao et al. quantitatively forecast the critical materials requirements in scenarios of high penetration of wind power in Denmark [18]. Deetman et al. performed a similar analysis on a global scale and extended to the whole electricity sector, showing a strong demand growth of the majority of the metals considered [19].

Moreover, traditional life-cycle-assessment (LCA) approaches is another method included in the boundaries of the analysed studies. It is the case of Stropnik et al., which assessed the criticality of raw materials for the production of PEMFC by means of classical LCA approaches, showing the relevant impact of recycling of end-of-life (EoL) technologies [20]. Building upon LCA, Motoori et al. adopted input-output analysis (IOA) to evaluate the impact of future decarbonization scenarios on the mining sector of Japan [21].

Drawing from the above-mentioned and described papers, different criticalities can be identified. While most of the studies investigate the effects of the energy transition on the consumption of critical raw materials, the majority of them mostly focus on few, and sometimes very peculiar, technologies that may be deployed in specific regions, without tracking multi-regional trade patterns. Moreover, non-negligible macroscopic trends such as the population growth or the direct effect of national or international policies on the energy sector (i.e. change in electricity production mix) are often not accounted for, often due to lack of available data or because of the methodology selection which may not be suitable for tracking such complexities. Providing a flexible tool to perform this kind of analyses configures as a possible solution to solve these issues.

In order to capture further studies focusing on proposing structured modelling frameworks to cover the highlighted features, the borders of the literature research have been extended. Concerning industrial ecology, one of the main research stream on the topic is the waste input-output (WIO) analysis. Nakamura and Kondo, starting from the formulation of the very first WIO model [22], were able to formulate the dynamic WIO concept [23], which integrates the full characterization of material recycling processes from end-of-life (EoL) products within a traditional input-output table. As a complement of the original WIO model, a work from Lenzen and Reynolds extended such model from IOTs to supply-and-use tables (SUTs) [24]. Such mentioned frameworks require an extensive amount of empirical data, which are not always provided by statistical institutions. As one notable integrated assessment model developed within the EU H2020 program, the MEDEAS model is capable of providing scenario analysis grounded on a general equilibrium macroeconomic mechanism, integrated with a module specifically devoted to account for energy and materials consumptions [25]. Moreover, Pauliuk at al. presented the RECC model, which adopts a dynamic Material Flow Analysis (MFA) to link of the utilisation of fundamental services for human well-being to climate change effects, by tracking the material efficiency of such services [26]. In the end, Donati et al. developed another noticeable framework devoted to model circular economy scenarios named pycirk and based on input-output analysis [27].

1.2. Aim of the work

This paper presents the DYNamic Extraction and Recycling Input-Output (DYNERIO) modelling framework, useful to assess the economic and environmental impacts of future scenarios in a multi-regional setting, focusing on critical materials supply chains relevant for the energy transition, and quantifying the related materials extraction and recycling in future scenarios.

The developed framework may represent a solution to the criticalities highlighted in the literature review and presents the following features. First, it is Python-based and open-source, hence characterised by high levels of flexibility and user-friendliness, aiming at reproducibility and transparency of scenario results. Secondly, the input-output structure of DYNERIO allows for a comprehensive understanding of the global materials metabolism via the implementation of a variety of scenarios in multiple industries, possibly extending its application also to non-energy-related ones. Finally, DYNERIO is suitable to couple both forecasting of materials demand and analysing impact of recycling practices.

To illustrate the novelties and possibilities brought by the proposed framework, a demonstrative case study is performed: the application is based on real macroeconomic and technical empirical data, and assumptions for the analysed scenarios are based on the outcomes of World Energy Outlook 2020 by IEA.

The paper is structured as follows: section 2 provides a presentation of the mathematical structure of the proposed framework. The case-study, describing the setting of the scenarios along with the related assumptions, is presented in section 3, while section 4 discusses the results obtained describing the advantages and limitations of the presented framework.

2. Methods and models

The DYNERIO framework is composed of two soft-linked modules, each devoted to specific tasks, as illustrated by Figure 1. Specifically, the Module 1 consists in a Multi-Regional Input-Output (MRIO) table when the basic principles of Leontief models are applied using consequential (shock) analyses: beside its underlying empirical dataset, in this module exogenously defined scenarios are implemented, based on future population trends, living standards and prospective technology changes (e.g. changes in regional energy mix), hence deriving regional and sectoral impact indicators (value added generation, energy use, emissions, etc.) and the related goods and services production yields, including the amount of energy carriers and services (e.g. transport service, electricity, heat, etc.).

Module 2 consists in a system of algebraic difference equations modelling the regional operation of supply chains of critical materials and the ones devoted to the production of the related energy systems. Such module receives information about the total capacity of technologies requested to be manufactured by each region, and determines, based on technical data related to the supply chains of critical materials and the related energy technologies, endogenously returns quantities of critical materials extracted, recycled and traded among regions in the analysed scenario.

The two core modules are linked via a *bridge calculation core* dedicated to calculate the technology installed capacity in the analysed time horizon to be fed to Module 2, starting from results in terms of energy services production which come as output of Module 1. Such bridge algorithm is shaped as an energy system linear programming optimization model.

The type of exogenous data to be delivered to the two Modules depends on the scope and level of detail requested by the scenarios under investigation, while energy transition scenarios are exogenously provided in the form of region- and sector-specific pathways for technology changes. For example, investigating the amount of neodymium requested for delivering wind energy in future scenarios calls for the disaggregation of wind power technology in the Module 1, while Module 2 requires an average technical characterization of wind power technology in terms of performance, energy availability, neodymium content per unit of installed capacity and recycling rates, the geographical localization of neodymium extraction and recycling activities and production/operation/disposal of the wind power technology.

In the following, the basic mathematical structure of the two modules is described, together with the basic assumptions and the characteristic modelling underlying features. A small-scale simplified conceptual model is provided in a spreadsheet as supplementary electronic material.

The next Figure depicts in the end a schematic representation of the DYNERIO framework highlighting the information exchange between its core and modules.

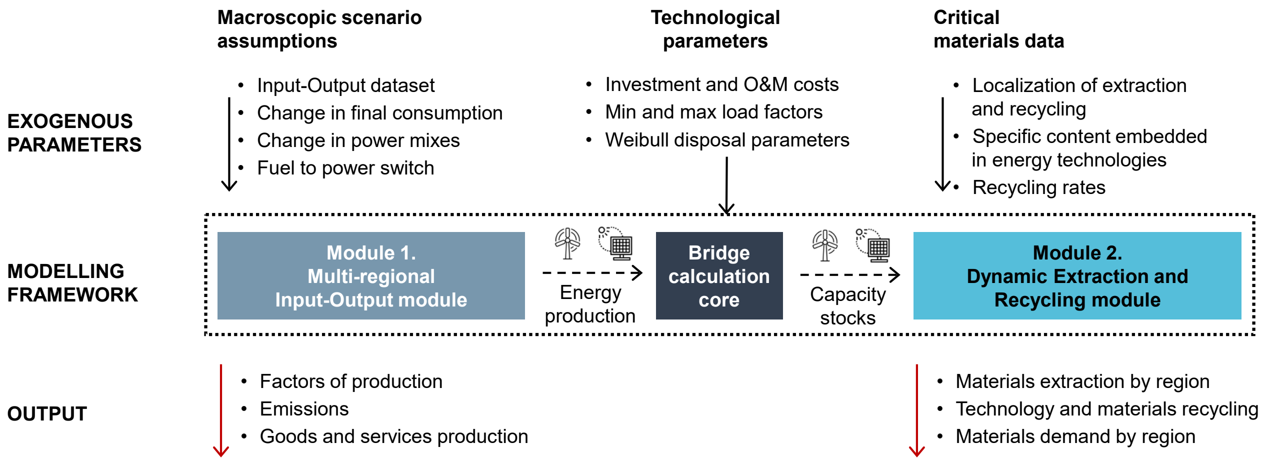

Figure 1. Schematic representation of the DYNERIO framework

2.1. Multi-Regional Input-Output module

The Module 1 is built upon empirical meso-economic datasets representing highly disaggregated national economic and environmental accounts, identifying flows of goods and services across industries in national and international economies. The basic mathematical structure reflects the classic Leontief representation of a multi-regional cluster of economies, here defined based on a symmetric input-output tables [28], resulting in a system of equations formulated by means of vectorial exogenous and endogenous variables listed in Table 1.

The model is defined by intermediate, final and exogenous transactions matrices (the latter distinguished as economic factors of production and environmental extensions), resembling data related to a baseline year (subscript $y = 0$ in Table 1). Such tables are derived based on available multi-regional or global input-output databases, either defined based on monetary or hybrid units: examples of widely adopted global databases are Exiobase, WIOD or Eora, revised by Owen in [29] and less recently by Wiedmann et al. in [30]. Selection of the appropriate dataset depends on the scenario analysis to be performed, and the related regional and sectoral coverages.

Table 1. Exogenous and endogenous parameters of the MRIO module. Notice that time step $y = 0$ refers to the baseline year (i.e. available data from national accounts), while $y > 0$ refers to years defined by scenarios' projection and y refers to all modelling years.

Category	Symbol	Size	Description
Indices	r		Regions
	n		Sectors per region
	k		Factors of production (capital, labour compensation, taxes, …)
	c		Final consumption categories (households demand, investments, …)
	e		Exogenous transactions categories (energy use, emissions, …)
	y		Time steps for the scenarios (years)
Exogenous variables	$\mathbf{Z}_{y=0}$	$rn \times rn$	Intersectoral transactions matrix (baseline year)
	$\mathbf{V}_{y=0}$	$k \times rn$	Factors of production matrix (baseline year)
	$\mathbf{E}_{y=0}$	$e \times rn$	Environmental transactions matrix (baseline year)

	$\mathbf{x}_{y=0}$	$rn \times 1$	Total production vector (baseline year)
	$\mathbf{Y}_y$	$rn \times rc$	Final demand matrix (all years)
	$\mathbf{z}_y$	$rn \times rn$	Intersectoral technical coefficients matrix (all years)
	$\mathbf{v}_y$	$k \times rn$	Factors of production coefficients matrix (all years)
	$\mathbf{e}_y$	$e \times rn$	Environmental transactions coeff. matrix (all years)
	$\mathbf{I}$	$rn \times rn$	Identity matrix
Endogenous variables	$\mathbf{x}_{y>0}$	$rn \times 1$	Total production vector (scenarios' projection)
	$\mathbf{Z}_{y>0}$	$rn \times rn$	Multi-regional transaction matrix (scenarios' projection)
	$\mathbf{V}_{y>0}$	$k \times rn$	Factors of production coefficients matrix (scenarios' projection)
	$\mathbf{E}_{y>0}$	$e \times rn$	Environmental transactions matrix (scenarios' projection)

Technologies already included in the intermediate transaction matrix may need to be further disaggregated to adequately represent the transition scenario and to allow the assessment of technology-specific requirements of critical materials: for example, if the assessment of rare hearts for magnet productions used in wind turbines is required, technologies included in regional power sectors need to be highly disaggregated. The same holds for other technologies, such as transport, heating and fuel production. Moreover, since input-output datasets collects data related to transactions of marketed products (also named commodity flows), the selected database may need to be elaborated by the user to disaggregate specific technologies or to endogenize them into the transactions tables. For example, mobility of households based on light duty passenger vehicles is not registered as a service in the IOT, that only accounts for consumption of fuel and the investment in vehicle acquisition as final demand items. Therefore, the standard database should be elaborated to embed vehicles powertrains (traditional internal combustion engines as well as and innovative one like electric powertrains) within the IOT as new technologies.

Once the IOT dataset related to the baseline year has been properly elaborated to reflect the needed technology disaggregation, total production in the baseline year is derived based on equation (1), where $\mathbf{i}$ is the summation vector of appropriate dimensions.

$$y = 0: \;\; \mathbf{x} = \mathbf{Z}\,\mathbf{i} + \mathbf{Y}\,\mathbf{i} \tag{1}$$

Coefficients tables for the baseline year are derived: intersectoral technical coefficients (2), factors of production coefficients (3), intermediate and final environmental transactions (4). Notice that final environmental transactions are derived as function of final consumption of domestically produced and imported commodities for every region (e.g. air emissions from final fuels consumption are originated both by domestically produced and imported fuels).

$$y = 0: \;\; \mathbf{z} = \mathbf{Z}\,\hat{\mathbf{x}}^{-1} \tag{2}$$

$$y = 0: \;\; \mathbf{v} = \mathbf{V}\,\hat{\mathbf{x}}^{-1} \tag{3}$$

$$y = 0: \;\; \mathbf{e} = \mathbf{E}\,\hat{\mathbf{x}}^{-1} \tag{4}$$

Such coefficients tables are then modified based on exogenous scenario data to represent future shifts in technology, trades, and change in final consumption yields and habits for the generic year $y > 0$ based on equation (5).

$$\left(\mathbf{z},\mathbf{v},\mathbf{e},\mathbf{Y}\right)_y = \left(\mathbf{z},\mathbf{v},\mathbf{e},\mathbf{Y}\right)_{y-1} + \Delta\left(\mathbf{z},\mathbf{v},\mathbf{e},\mathbf{Y}\right)_y \tag{5}$$

Finally, the models' endogenous parameters can be derived: total production vector (6), intersectoral transactions (7), factors of production (8), and intermediate and final environmental transactions (9) and (10). Notice that final environmental transactions are derived based on scalar multiplication of the related coefficients and the final domestic and imported demand of products.

$$y > 0: \ \mathbf{x} = \left(\mathbf{I} - \mathbf{z}\right)^{-1} \mathbf{Y}\mathbf{i} \tag{6}$$

$$y > 0: \ \mathbf{Z} = \mathbf{z}\,\hat{\mathbf{x}} \tag{7}$$

$$y > 0: \ \mathbf{V} = \mathbf{v}\,\hat{\mathbf{x}} \tag{8}$$

$$y > 0: \ \mathbf{E} = \mathbf{e}\,\hat{\mathbf{x}} \tag{9}$$

Regarding scenarios projections, few important remarks are in order. First, since the proposed IO model is not a dynamic model as descripted by Miller and Blair [28], adequate assumptions are required to deal with investments by region, the impact of which may not be negligible [31]. One solution may be to define and to project sectoral investments by region based on reliable scenario assumptions. Another approach may consists in embedding investments and fixed capital consumption (respectively collected within final demand and factor inputs matrices) in the intermediate transaction tables, relying on approaches descripted by Lenzen et al. [32], [33].

Secondly, due to the fact that technology shifts are exogenously assumed by the model, a non-productive technology coefficients matrix may be returned by equation (6): system productivity must be therefore checked in every time step. Among the variety of available approaches, Duchin and Levine recently proposed an approach based on linear programming technique which can be also applied for hybrid units databases [34].

2.2. Bridge calculation core

As mentioned at the beginning of the section, the soft link between the two modules is performed via a bridge calculation core algorithm defined by an optimization linear programming energy model.

Table 2. Exogenous and endogenous parameters of the bridge calculation algorithm.

Category	Symbol	Size	Description
	r		Regions
Indices	t		Technologies
	y		Time steps for the scenarios (years)
	$\mathbf{y}$		Time steps vector defining by a sequence of all the time steps

Exogenous variables	$\mathbf{x}_{rt}$	$rt \times rt$	Total production vectors of selected technologies (one for each year)
	$\mathbf{c}_{op}$	$rt \times 1$	Specific operation costs per unit of production
	$\mathbf{c}_{inv}$	$rt \times 1$	Specific investment costs per unit of capacity
	d		Discount rate
	β	$t \times 1$	Weibull shape factor defined by technology
	l	$t \times 1$	Technical lifetime defined by technology
	l_{res}	$t \times 1$	Residual technical lifetime at year 0, defined by technology
	$\mathbf{K}_{ope,y=0}$	$rt \times y$	Operative capacity in the first time step
	$\mathbf{A}_{min}$	$t \times 1$	Minimum technologies availability
	$\mathbf{A}_{max}$	$t \times 1$	Maximum technologies availability
Endogenous variables	$\mathbf{Cd}$	$rt \times y$	Total discounted costs
	$\mathbf{C}$	$rt \times y$	Total undiscounted costs
	$\mathbf{C}_{op}$	$rt \times y$	Operation costs
	$\mathbf{C}_{inv}$	$rt \times y$	Investment costs
	$\mathbf{K}_{ope,y>0}$	$rt \times y$	Operative capacity after the first time step
	$\mathbf{K}_{new}$	$rt \times y$	New installed capacity
	$\mathbf{K}_{disp}$	$rt \times y$	Total disposed capacity
	$\mathbf{K}_{disp(y=0)}$	$rt \times y$	Disposed capacity out of the operative capacity installed at year 0
	$\mathbf{K}_{disp(y>0)}$	$rt \times y$	Disposed capacity out of the operative capacity installed after year 0
	$\mathbf{A}_{real}$	$rt \times 1$	Actual technologies availability

The objective function of the model is the minimization of the net present cost of investment and operation of the new and already existing technology capacity required to fulfil the energy service production (10).

$$\text{Obj Function: } Min\, Z = \mathbf{i}_{1,rt}\mathbf{Cd}\,\mathbf{i}_{y,1} \tag{10}$$

In this function $\mathbf{Cd}$ indicates the total discounted costs, determined by the regional discount rate d, defined in equation (11),

$$\mathbf{CD} = \frac{\mathbf{C}}{(1+d)^{y-1}} \tag{11}$$

where $\mathbf{C}$ is given by the sum of investment and operative costs required for the installation, operation and maintenance of the new and operating capacities in each region and for each technology (12).

$$\mathbf{C} = \mathbf{C}_{inv} + \mathbf{C}_{op} \tag{12}$$

As said, the investment cost is related to the new capacity to be installed $\mathbf{K}_{new}$, while the operative cost is linked to the operating capacity $\mathbf{K}_{ope}$, as defined by equations (13) and (14), where also the specific investment ($\mathbf{c}_{inv}$) and operation costs ($\mathbf{c}_{op}$) , expressed per unit of technology capacity and technology output ($\mathbf{x}_{rt}$) respectively, are introduced.

$$\mathbf{C}_{inv,rt} = \mathbf{K}_{new,rt}\mathbf{c}_{inv,rt} \tag{13}$$

$$\mathbf{C}_{op,rt} = \mathbf{x}_{rt}^{\mathrm{T}}\hat{\mathbf{c}}_{op,rt} \tag{14}$$

New and operating capacities are strictly interconnected since, for each year, the capacity balance equation (15) needs to be respected. In particular, the operating capacity of each year is given by the one of the year before at the net of the capacity disposed at its end of life plus the capacity which is newly installed to counterbalance such disposal and fulfil the future energy needs.

$$\begin{cases} \mathbf{K}_{ope,y=0} = \text{exogenous parameter } (y=0) \\ \mathbf{K}_{ope,y>0} = \mathbf{K}_{ope,y-1} + \mathbf{K}_{new,y} + \mathbf{K}_{disp,y} \end{cases} \tag{14}$$

The total disposed capacity $\mathbf{K}_{disp}$ calculation (15) is performed in two steps: (i) first it is requested to calculate the yearly capacity disposal of the operating capacity present since the first year ($\mathbf{K}_{disp(y=0)}$), which is assumed to have a residual lifetime of l_{res}; (ii) the second term calculates the disposal of the capacity which is installed in the future years ($\mathbf{K}_{disp(y>0)}$).

$$\mathbf{K}_{disp} = \mathbf{K}_{disp,(y=0)} + \mathbf{K}_{disp,(y>0)} \tag{15}$$

These latter two terms are both calculated as the sum of the yearly disposed capacities following a Weibull distribution function based on the technical lifetime of each technology l and having a technology-specific shape factor β, as described by equation (16).

$$\begin{cases} \mathbf{K}_{disp,(y=0)_y} = \mathbf{K}_{ope,y=0} \cdot \left[1 - e^{-\left(\frac{y+l_{res,y=0}}{\beta_t}\right)^l} \right] \\ \mathbf{K}_{disp,(y>0)} = 0 \quad (y=0) \\ \mathbf{K}_{disp,(y>0)_{r,t,y}} = \left[1 - e^{-\left(\frac{y}{\beta_t}\right)^l} \right] \mathbf{K}_{new_{r,t,y}} \quad (y>0) \end{cases} \tag{16}$$

An additional constraint to be considered in the model, as the energy service production is taken exogenously from the MRIO module, is given by the technical range of operation which each technology should respect, given by the minimum and maximum availabilities ($\mathbf{A}_{min}$, $\mathbf{A}_{max}$)

$$\mathbf{A}_{\min_{r,t}} \leq \mathbf{A}_{r,t} \leq \mathbf{A}_{\max_{r,t}} \tag{17}$$

2.3. Dynamic Extraction and Recycling module

Starting from known values of newly installed and disposed technology capacities obtained by the bridge calculation core, the Dynamic Extraction and Recycling (dynER) module is finally in charge of assessing the amount of materials requested and extracted in each region at the net of the recycling availability.

Table 3. Exogenous and endogenous parameters of the Dynamic Extraction and Recycling module

Category	Symbol	Size	Description
	r		Regions
	p		Regions manufacturing technologies
Indices	t		Technologies
	m		Materials
	y		Time steps for the scenarios (years)

Exogenous variables	$\mathbf{M}_c$	$t \times m$	Material content by technology and region
	$\mathbf{K}_{new}$	$rt \times y$	New installed capacity
	$\mathbf{K}_{disp}$	$rt \times y$	Total disposed capacity
	$\mathbf{T_S}$	$rt \times p$	Technologies manufacturing shares, by region
	$\mathbf{M}_{R,R}$	$r \times m$	Material recycling rates, by region
	$\mathbf{T}_{R,R}$	$rt \times 1$	Technologies recycling rates, by region
	$\mathbf{M}_E$	$r \times m$	Material extraction shares, by region
Endogenous variables	$\mathbf{T_P}$	$rt \times y$	Technology production by region
	$\mathbf{D}_{gross}$	$rm \times y$	Gross materials demand, by region
	$\mathbf{T_R}$	$rt \times y$	Technology capacity recycled by region
	$\mathbf{M_R}$	$rm \times y$	Recycled materials, by region
	$\mathbf{D}_{\boldsymbol{net}}$	$rm \times y$	Net materials demand, by region
	$\mathbf{D}_{net,global}$	$m \times y$	Net materials demand, global
	$\mathbf{Ex}$	$rm \times y$	Demand extraction, by region

By providing the manufacturing shares of each technology by each region ($\mathbf{T_S}$), the dynER module allows to calculate the actual production of technology requested to each region $\mathbf{T_P}$, by multiplying the capacity to be installed in each region by $\mathbf{T_S}$ (18):

$$\mathbf{T}_{\mathbf{P}_{r,t,y}} = \sum_{p} \left(\mathbf{K}_{new_{r,t,y}} \cdot \mathbf{T}_{\mathbf{S}_{r,t,p,y}} \right) \tag{18}$$

From $\mathbf{T_P}$, as a straight consequence, it is possible to derive the total material required by the manufacturing technologies ($\mathbf{D}_{gross}$):, by knowing information about the material content of each technology ($\mathbf{M}_c$):

$$\mathbf{D}_{gross} = \mathbf{T_P} \cdot \mathbf{M_C} \tag{19}$$

Such gross demand of materials needs to be reduced by the amount of materials which are going to be recycled (which depends on the recycling rate of each technology in each region ($\mathbf{T}_{RR}$), as described by equation (20)), leading to the net materials demand of each region $\mathbf{D}_{net}$ (21).

$$\mathbf{T_R} = \mathbf{K}_{disp} \cdot \mathbf{M}_{R,R} \tag{20}$$

$$\mathbf{D}_{net} = \mathbf{D}_{gross} - \mathbf{T_R} \tag{21}$$

By summing $\mathbf{D}_{net}$ region by region, the global demand of each material can be derived as $\mathbf{D}_{net,global}$, which is multiplied by the materials extraction share matrix $\mathbf{M}_E$ to calculate the actual material extracted in each region $\mathbf{Ex}$ (22):

$$\mathbf{Ex} = \mathbf{D}_{net,global}\ \mathbf{M}_{\mathbf{E}}^{\mathbf{T}} \tag{22}$$

3. Case study description

A simplified case study was developed as a demonstrative example. The whole set of input data assumed, the high-resolution charts, along with a conceptual Excel file is available on the Github repository dedicated to this paper [35], serving as a reproduceable first-try structured application of the approach. Furthermore, the core DYNERIO code is integrated within the MARIO framework for more advanced applications.

For this case study, a simplified energy transition pathway as been modelled based on the following assumptions. Starting by the hybrid version of the Exiobase database [36], the world has been aggregated in two regions, namely the OECD countries (which are represented, in terms of policies implemented by European Union) and the Rest of the World (RoW). Economic activities have been aggregated in 4 macro-activities: goods and services, fossil fuels and products, electricity by non-renewables, electricity by renewables. The supply-use database has been transformed into a product-by-product input-output tables by adopting the methodology reported by the Eurostat manual on supply-use input-output tables [37].

The energy transition pathway in driven by three main phenomena:

- Change in final demand: each region's final demand is expected to increase according to increase of living standards and population growth. This information are elaborated based on World Bank and UN population division datasets.
- Change in power production mix: based on IEA World Energy Outlook 2021 Sustainable Development scenario [38], OECD and RoW will change their production mix of electricity shifting towards a large renewable penetration. Assuming a linear increase of such penetration an yearly switch of 25.6% and 23.2% from non-renewables to renewables has been applied in power mixes of OECD and RoW respectively.
- Fuels to power switch: a progressive switch from fossil fuels adoption towards electricity consumption has been modelled in all sectors: respectively 10% of fossil fuels and related products per year are modelled to be replaced by electricity consumption in OECD, while 8% in RoW. Since consuming a different fuel implies consuming energy with a different efficiency, a factor of 1.8 (OECD) and 1.5 (RoW) have been considered when shifting from fossil to electricity-based technologies.

The starting table has been assumed to represent a conceptual representation of year 2020, and has been replicated in the MRIO module other nine times in order to model the transition pathway up to 2070 with a time step of 5 years.

As discussed in the previous section, further exogenous parameters are necessary to the other modules. *Electricity by non-renewables* technologies have been assumed to operate within a range of 30% and 90% of their nominal capacity, while the *Electricity by renewables* technologies are assumed to operate at a constant 30% load factor in both regions ($\mathbf{A}_{min}$, $\mathbf{A}_{max}$). For the former, a 30 years lifetime was assumed, while 20 years were considered for the latter. The already existing operating capacity is assumed to be in the middle of its technical lifetime (l_{res}). Regarding specific costs of installation and operation, the main assumptions are reported in the following table.

Table 4. Specific investment and operation costs by technology

			Electricity by non-renewables	Electricity by renewables
Specific operation costs	$\mathbf{c}_{op}$	M€/TWh	0.1	0
Specific investment costs	$\mathbf{c}_{inv}$	M€/GW	600	1500

Regarding the dynER module, the first information requested is the share of manufacturing of technologies by each region ($\mathbf{T_S}$): given the Chinese monopoly in the production of renewables technology, the production of such technologies has been assumed to be totally located in RoW apart from OECD covering 10% of its domestic needs. About fossil-fired electricity production plants, each region has been assumed to supply 70% of its domestic demand and to import 30% from abroad. For both technologies, a 50% recycling rate has been assumed without making regional distinctions.

Two selected materials necessary for wind turbines and PV panels production, has been selected for the analysis: (i) silicon (Si) is a fundamental resource in the supply chain of PV panels which contains around 35 tonnes per GW installed according to the reference and the PV technology [7]; (ii) neodymium (Nd) is instead crucial for permanent magnets production, vastly adopted in wind turbines, which are estimated to contain on average 30 tonnes per GW of neodymium. Null consumption of such materials is assumed for non-renewables technologies. While neodymium recycling rate has been approximated at 5% and 2.5% in OECD and RoW respectively [39], silicon's one was assumed as 10% [40]. The two minerals were estimated to be extracted for 5% in OECD and 95% in RoW.

4. Results

The modelling framework can provide a suite of results, and this section aims at giving a compact and comprehensive overview of them. As it was stated previously, the case study has to be intended as a demonstrative example, without claiming of providing realistic results.

The results dashboard (which can be visualized extensively in the DYNERIO_concept excel file in the Github repository at [35]) shows an extensive suite of heterogeneous outputs determined by the multifaceted nature of the integrated framework. From the MRIO module, it is possible to derive the raising trend in electricity generation which can be compared with fossil fuels production decrease due to the scenario assumptions provided (Figure 2).

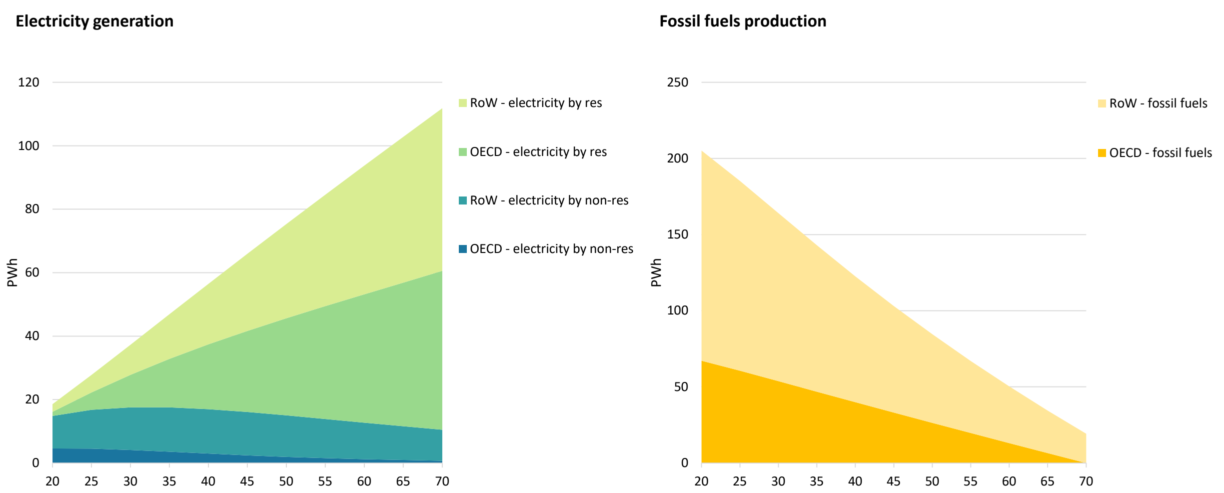

Figure 2. Electricity and fossil fuels production in OECD and RoW. Time horizon is the 2020-2070 period

Another interesting macro result, fundamental when dealing with energy transition pathways analysis, CO2 emissions, both in absolute values and in terms of emission intensity per unit of GDP can be derived as shown in Figure 3.

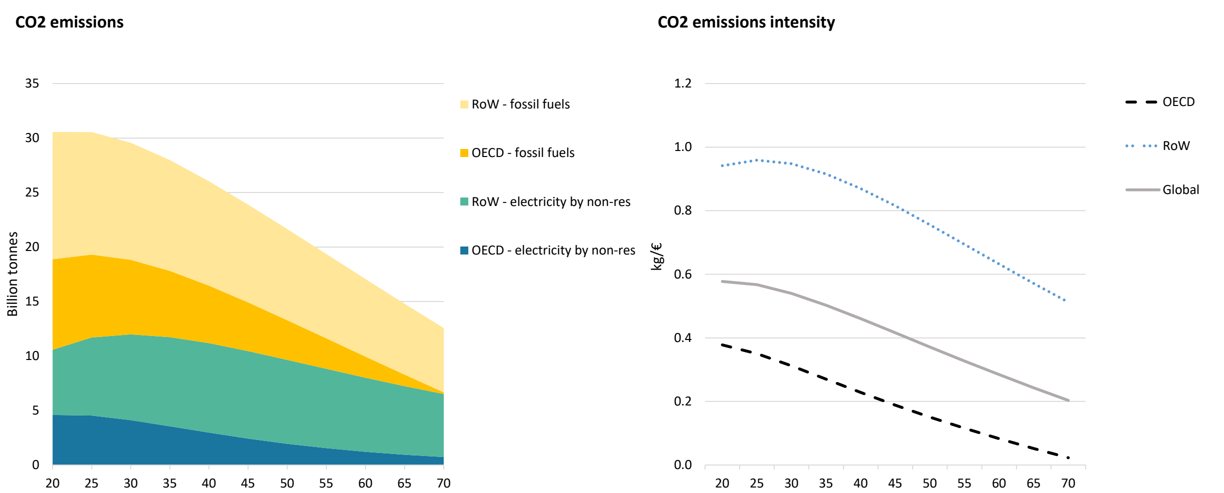

Figure 3. CO2 emissions: absolute and per unit of GDP. Time horizon is the 2020-2070 period

The bridge calculation core instead, as mentioned in the methodological section, is in charge of computing the new and disposed capacity by year, which can be expressed in terms of non renewables and renewables plants in our simplified approach. Figure 4 shows such trend by highlighting in the negative side of the vertical axis the disposed capacity while the newly installed capacity on the positive side.

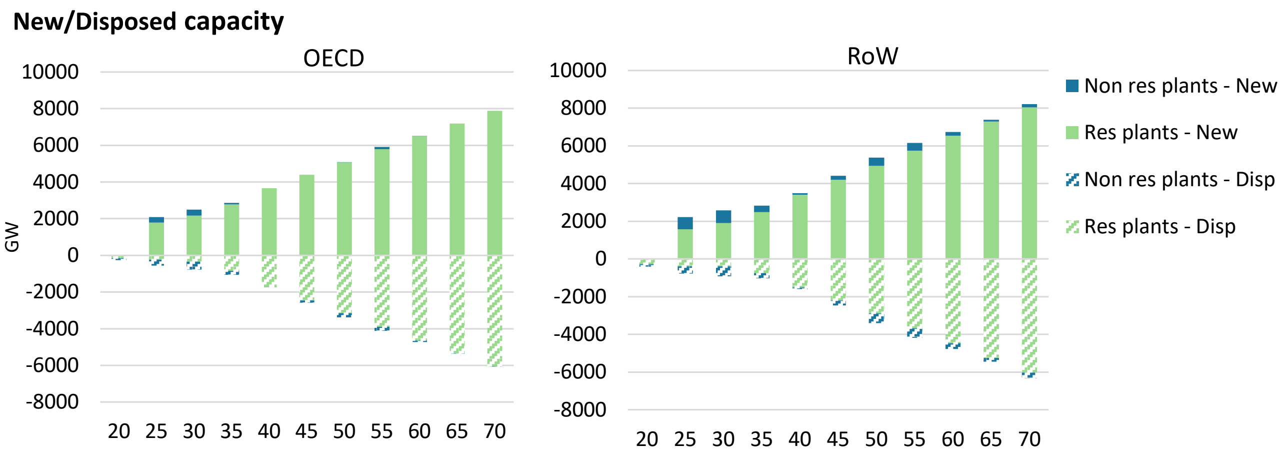

Figure 4. New and disposed capacity by year from 2020 to 2070 in OECD (left) and RoW (right). The negative side of the vertical axis shows the disposed capacity while the newly installed capacity is located on the positive side. Note the scales for the two regions are different.

Coming to the dynER module, it is possible to notice that depending on the attitude towards materials recycling and the localization of materials extraction, the results may differ a lot between the two regions, as shown in Figure 5 and Figure 6.

Figure 5 shows the total amount of materials embedded in the demand of renewables technology manufacturing sectors (in light blue) and the recycled amount of materials recovered from the end of life of such technologies (in dark blue). It is evident that, at least in the very short term, due to the small portion of capacity stock shared by the renewable energy power plants nowadays, the effect of recycling is negligible: while in RoW recycling is not appreciable even in 2070 due to the very low recycling rates and the very high demand of materials coming from domestic and foreign needs, in OECD the net demand is diverging significantly from the gross demand only after 2050. This implies that unless striving innovation disrupts in the recycling processes of such materials, recycling itself may not be a viable solution to decrease materials demand by mid-century.

Figure 6 instead focuses on the amount of materials extracted in each region: due to the strong unbalance in this parameter towards the RoW due to the physical location of the actually exploitable mineral resources, the large majority of the materials is expected to be extracted in this latter region.

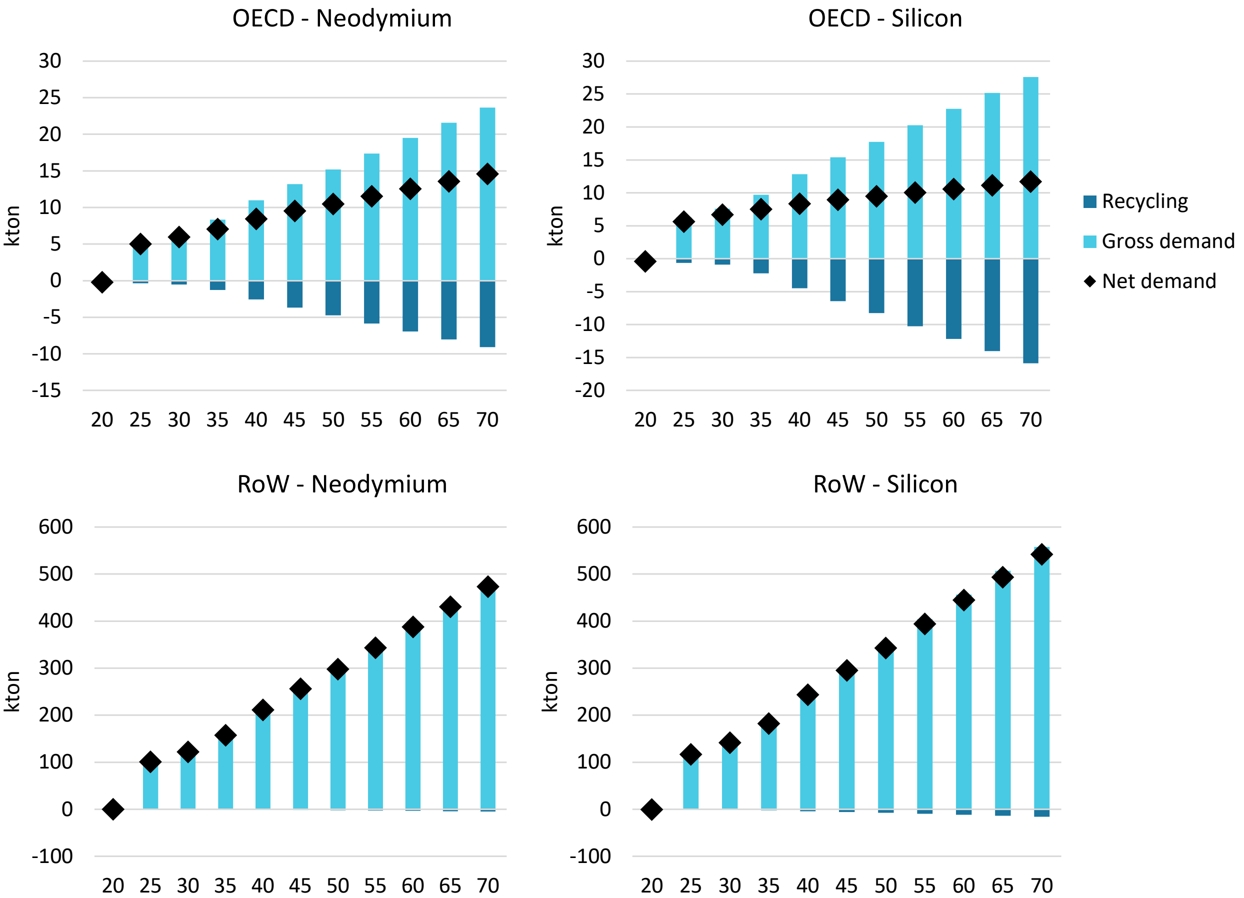

Figure 5. Materials demand and recycling driven by technology manufacturing purposed by region.

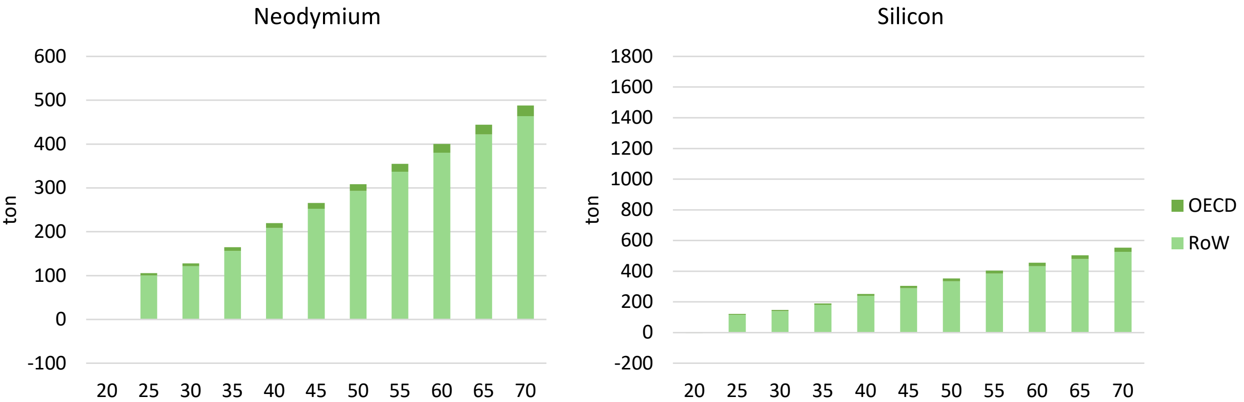

Figure 6. Materials extraction by region and year

5. Discussion and conclusions

The work provides a presentation of a novel framework for critical material analysis based on input-output analysis. The presented framework is in compliance with all the current state of the art modelling features and properties which have been highlighted in the literature review. It both allows to assess and quantify the demand of critical materials according to a given scenario and, at the same time, it provides insights on the impact of circular economy practices put in place to mitigate the intensity of material extraction processes envisaged by the implemented scenarios.

The framework results also to be very flexible and versatile to the users' needs, allowing for the implementation of a variety of energy- and non-energy-related macroscopic scenarios and trends, which is a typical characteristics of input-output models given the vast sectoral scope that characterises the underlying datasets. Furthermore, the impact of the implemented scenarios on the materials extraction and recycling can be investigated in a detailed and customisable manner, starting from the selection of the desired relevant technologies, which may be extended also to the non-energy-related ones (such as electronics, manufacturing processes…), and the selection of the materials embedded in such technologies.

The suite of results that can be obtained is complete of both macroeconomic and environmental indicators, which may be extended by the user during the set-up phase of the input-output database, providing the desired satellite accounts in terms of emissions, energy use, employment rate, water and land consumption, according to the available data embedded in the MRIO database adopted. The results are also complete with a sensitivity analysis module, which allows for comprehensive scenarios comparisons.

The framework presents also some evident limitations. In the first place, the definition of the scenarios is fully exogenous and the whole procedure of performing the impact evaluation is deeply data intensive. The analyst needs therefore to provide accurate data starting from the MRIO database, and moving to the load factors, the material intensity data of the technologies, the regional localization of the extraction practices and the recycling rates. In case of high inaccuracy of the input data, the results will not be reliable.

The second major limitation is related to the first one and can be addressed to the purely simulation nature of the model. The technological pathways must be provided exogenously and no objectives or targets to be matched can be set. The complexities of switching the framework into an optimisation model are not negligible both from the conceptual and from the practical points of view, since there are not many consolidated examples of optimization input-output models. However the authors are going in this direction for a further development of this work.

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