ENhancing our understanding of Trade Impacts on Climate, industries, and the Environment

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D2.4 – Enhanced GTAP Database

WP2 – Improved data and empirics on trade and climate

30/06/2026

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EC Summary Requirements

1. Changes with respect to the DoA

No changes with respect to the work described in the DoA.

2. Dissemination and uptake

Data collections and database disaggregation routines accompanying this report will be used to develop the enhanced version of the Global Trade Analysis Project (GTAP) Data Base, which will serve as a core input to the models within the ENTICE project. In addition, both data collections and data reconciliation algorithms accompanying this report can be used for the disaggregation of other global economic databases and for the enhancement of the multi-sectoral global and regional modelling frameworks (e.g. computable general equilibrium and integrated assessment models).

3. Short summary of results (<250 words)

The deliverable focuses on the enhancement of the Global Trade Analysis Project (GTAP) Data Base in the part of energy-intensive sectors, describing the first release of sectoral inventories required to extend the GTAP multi-regional input-output (MRIO) database in support of the modelling activities undertaken within the ENTICE project. The deliverable accompanies the sector-level data inventories necessary for the disaggregation and expansion of the GTAP-Power v12a database (with 2023 reference year), enabling a more detailed representation of industrial activities relevant to the analysis of trade, climate, and industrial transformation policies. The inventories are delivered in a standardized format that allow to reproduce the database extensions within the Multifunctional Analysis of Regions through Input-Output (MARIO) framework, supporting automated integration into the database construction workflow while preserving the aggregate consistency of the underlying GTAP database.

4. Evidence of accomplishment

This report, together with the accompanying sector inventories and the open-source disaggregation routine. The disaggregation model and the guided example are publicly available on GitHub (https://github.com/it-is-me-mario/MRIO-disaggregation-model); the underlying data inventories are released through the project's Zenodo community (DOI: https://doi.org/10.5281/zenodo.20592035).

Preface

In today's interconnected global economy, understanding the trade-climate nexus is more critical than ever. Trade policies significantly influence environmental outcomes, while climate change affects trade flows. However, the complex relationship between these areas remains insufficiently explored, often due to data limitations, gaps in economic modeling and the evolving nature of global supply chains. The ENTICE project aims to bridge these knowledge gaps by advancing our understanding of the trade-climate-industry (TCI) nexus. It examines how trade policies impact environmental sustainability and how climate policies shape global trade dynamics. By developing fact-based insights and innovative modeling tools, ENTICE supports informed decision-making at this crucial intersection of trade, climate, and sustainability.

E3M – E3-MODELLING AE	EL	
CMCC – FONDAZIONE CENTRO EURO-MEDITERRANEOSUI CAMBIAMENTI CLIMATICI	IT	
WI – WUPPERTAL INSTITUT FUR KLIMA, UMWELT, ENERGIE GGMBH	DE	
REFORM – FUNDACJA INSTYTUT REFORM	PL	
VUA – STICHTING VU	NL	
HOL – HOLISTIC IKE	EL	
ENEXTGEN – ENEXTGEN S.R.L.	IT	
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1 Introduction

Global economic models, such as computable general equilibrium and integrated assessment frameworks, are widely used for the quantitative analysis of trade, climate, and industrial policies. While being well-suited for assessing economic impacts and identifying trade-offs across alternative policy solutions, these frameworks, however, are often criticized for the lack of sectoral granularity. The analytical resolution of these modelling frameworks is constrained by the underlying databases, which often being of the global nature are limited in their sectoral details essential to support the analysis of specific policy questions (e.g. technology-specific policies or mineral-level assessments). This limitation also applies to the Global Trade Analysis Project (GTAP) Data Base, which underlies most of the global CGE models (Aguiar et al., 2025). The latest version of the GTAP Data Base – version 12, while covering 163 countries and regions represents the economy using 65 sectors, with e.g. a single mineral mining activity.

Given the ENTICE project's objective of advancing the understanding of interactions between trade policies, climate impacts, mitigation strategies, and industrial transformation, the availability of granular and comprehensive data constitutes a critical foundation for credible modelling and accurate policy evaluation. Previous deliverables within the ENTICE project – particularly, deliverable 2.3 – identified specific data needs across key sectoral groups, including critical minerals (and related supply chains), energy-intensive and green technologies, agri-food sectors, land-use activities and international transportation, which should be addressed to advance the representation of the corresponding activities in the economy-wide models.

In the current deliverable we focus on the enhancement of the GTAP Data Base in the part of energy-intensive sectors. Thus, the objective of Deliverable D2.4 is to provide the first release of sectoral inventories required to extend the GTAP multi-regional input-output (MRIO) database in support of the modelling activities undertaken within the ENTICE project. The deliverable supplies the sector-level data necessary for the disaggregation and expansion of the GTAP-Power v12a database (with 2023 reference year), enabling a more detailed representation of industrial activities relevant to the analysis of trade, climate, and industrial transformation policies. The provided data collections support the disaggregation of 11 parent GTAP sectors into 81 new sectors.

The deliverable provides a set of structured sectoral inventories that can be used by authorised GTAP users to reproduce the database extensions within the MARIO framework (Tahavori et al., 2023). The inventories are delivered in a standardized format that supports automated integration into the database construction workflow while preserving the aggregate consistency of the underlying GTAP database. This deliverable constitutes the first stage of a broader data development effort under Work Package 2. Subsequent deliverables will further expand the database coverage, including agricultural and livestock sector data (D2.5), transport-related energy and emission accounts (D2.6), and a comprehensive refined dataset release aimed at supporting the development and implementation of the overall modelling activities within the ENTICE project (D2.8). Beyond its role within WP2, the deliverable also provides inputs to WP3, which focuses on advancing the capabilities of models used in the project. More precisely, the findings of this report are directly relevant to Task 3.2 *“Enhancing the sectoral disaggregation of models: EIIs, land use, transport sectors, clean technology manufacturing, and resources”* which aims to improve macroeconomic models by increasing their sectoral granularity.

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1.1 Structure of the report

The report is organised as follows. Section 2 defines the sectoral scope of the GTAP database extension developed in this deliverable. It identifies the original GTAP sectors selected for disaggregation and lists the new ENTICE sectors introduced, with particular attention to energy-intensive industries, critical raw materials, clean technologies, and related manufacturing activities.

Section 3 describes the delivered data package. It first presents the structure and format of the sectoral inventory files, explaining how the Excel workbooks are organised and how they are intended to be read by the MARIO-based disaggregation routine. It then documents the original data collection process, the main data sources used, and the assumptions applied to harmonise heterogeneous sectoral evidence into a consistent GTAP-compatible framework. The section further explains how the initial collection templates were transformed into final inventories, describes the disaggregation methodology and its implementation, and discusses the reconciliation and gap-filling procedures used to ensure consistency with the reference GTAP-Power v12a database. Finally, it reports the main quality assurance steps and the limitations of the current release.

Section 4 summarises the main conclusions of the deliverable and outlines the next steps towards the subsequent database releases planned within Work Package 2. These include the integration of additional sectoral domains, such as agriculture, livestock, transport, and the consolidated refined dataset supporting the modelling activities of the ENTICE project.

The Annex provides supplementary information supporting the delivered data package, while the Bibliography lists the references used for the construction and documentation of the inventories.

2 Sectoral scope

The sectorial detail of the GTAP database is being improved by disaggregating 11 existing sectors into 81, following the priorities outlined in Deliverable 2.3. The sector “Other mining extraction” is split into 18 sectors, “Petroleum, coal products” is split in 2, “Chemical products” into 19 sectors, “Rubber and plastic products” into 4 sectors, “Non-metallic minerals” into 3 sectors, “Iron and steel” into 7 sectors, “Non-Ferrous Metals: production and casting of copper, aluminium, zinc, lead, gold, and silver” into 11 sectors, “Computer, electronic and optical products” is split in 2, “Rest of Electrical equipment” into 7 sectors, “Motor vehicles and parts” into 6 sectors and “Transport nec” is split in 2. Table 1 presents the new proposed sectors with their denomination and 3-letter code, while the first two column report the belonging sector in the original GTAP database.

The disaggregation of sectors regarding agriculture and transportation are allocated to forthcoming deliverables, as reported in the "New sectors classification.xlsx" Excel file described in the Zenodo repository of this deliverable. Agricultural sectors data will be provided with D2.5 (New LULUCF matrix for GTAP) topics while transport data will be included in D2.6 (New transport matrix for GTAP).

Table 1. List of added sectors; sectors marked with * are computed as residuals so no individual inventory is included; sectors marked with ** will be included in next data releases

Parent GTAP sector code	Parent GTAP sector name	Sector code	Sector name
OXT	Other Mining Extraction	MAO	Mining of aluminium ores
		CHR	Mining of chromium
		COB	Mining of cobalt ores and concentrates
		MCU	Mining of copper ores
		MIO	Mining of iron ores
		LIT	Mining of lithium
		MAN	Mining of manganese ores and concentrates
		GRA	Mining of natural graphite
		MGC	Mining of natural magnesium carbonate "magnesite" and magnesia
		NIK	Mining of nickel ores and concentrates
		NIO	Mining of niobium
		PGM	Mining of platinum group metals
		REE	Mining of rare earth elements
		SIL	Mining of silver
		TIT	Mining of titanium
		MUR	Mining of uranium
		ZIN	Mining of zinc
		XOO	Mining of other ores*
P_C	Petroleum, coal products	PCP	Manufacture of coke
		PEP	Manufacture of petroleum products*
CHM	Chemical products	AMM	Manufacture of ammonia**

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Parent GTAP sector code	Parent GTAP sector name	Sector code	Sector name
		HYE	Manufacture of hydrogen via electrolysis
		HYS	Manufacture of hydrogen via steam reforming **
		HVC	Manufacture of high value chemicals
		MTH	Manufacture of methanol
		MSI	Manufacture of metallurgical silicon
		CRR	Manufacture of refined chromium
		COR	Manufacture of refined cobalt
		GAR	Manufacture of refined gallium
		LIR	Manufacture of refined lithium
		MNR	Manufacture of refined manganese
		NIR	Manufacture of refined nickel (chemical intermediates)
		RER	Manufacture of refined rare earths
		TIR	Manufacture of refined titanium
		ZIR	Manufacture of refined zinc
		NFR	Manufacture of nitrogen fertilizer
		PFR	Manufacture of phosphorus fertilizer
		KFR	Manufacture of potassium fertilizer
		XCH	Manufacture of other chemicals*
RPP	Rubber and plastic products	RBR	Manufacture of rubber products
		PLP	Manufacture of primary plastic products
		PLS	Manufacture of secondary plastic products
		PLR	Recycling of plastics
NMM	Non-metallic minerals	CEM	Manufacture of traditional cement
		AGT	Manufacture of artificial graphite
		NMX	Manufacture of other non-metallic minerals*
I_S	Iron and steel	SCI	Manufacture of steel via BF-BOF with coke injection
		SGI	Manufacture of steel via BF-BOF with natural gas injection
		SHI	Manufacture of steel via BF-BOF with hydrogen injection**
		SDH	Manufacture of steel via direct reduction with hydrogen
		SDG	Manufacture of steel via direct reduction with natural gas
		ISS	Manufacture of secondary iron and steel
		XIS	Manufacture of other iron and steel*
NFM	Non-Ferrous Metals: production and casting of	NFC	Casting of other non-ferrous metals
		APP	Manufacture of primary aluminum

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Parent GTAP sector code	Parent GTAP sector name	Sector code	Sector name
	copper, aluminium, zinc, lead, gold, and silver	APS	Manufacture of secondary aluminum
		RAL	Recycling of aluminum
		CPP	Manufacture of primary copper
		CPS	Manufacture of secondary copper
		RCP	Recycling of copper
		MUN	Manufacture of magnesium: unwrought, articles
		PGR	Manufacture of semi-manufactured platinum group metals
		SIR	Manufacture of refined silver
		NFX	Manufacture of other metals (primary, secondary and recycling)
ELE	Computer, electronic and optical products	SOP	Manufacture of solar panels
		XEL	Manufacture of computer, electronic and optical products*
EEQ	Rest of Electrical equipment	NCM	Manufacture of NCM batteries
		NCA	Manufacture of NCA batteries
		LFP	Manufacture of LFP batteries
		LCO	Manufacture of LCO batteries
		LMO	Manufacture of LMO batteries
		WNT	Manufacture of Wind turbines
		XEQ	Manufacture of other electrical equipment*
MVH	Motor vehicles and parts	ICH	Manufacture of heavy duty ICEV
		BVH	Manufacture of heavy duty BEV
		ICL	Manufacture of light duty ICEV
		HEL	Manufacture of light duty HEV
		BVL	Manufacture of light duty BEV
		XMV	Manufacture of rest of motor vehicles and parts*
OTP	Transport nec	TVP	Transport via pipeline service
		XTP	Other land transport*

Figure 1 summarises the scale and composition of the extension. For each parent GTAP sector listed in Table 1, it reports the global production and value added recorded in the reference GTAP-Power v12a database, broken down into the new ENTICE sectors split from that parent (legend); the hatched "Rest of ..." segment is the residual parent sector, i.e. the part of the original activity not reassigned to the new sectors. The relative weight of the new sectors differs markedly across parents - from cases where they account for most of the parent's output (e.g. petroleum and coal products, P_C) to cases where they isolate a smaller, policy-relevant share (e.g. chemicals, CHM). Because each parent sector is only redistributed internally, the bar totals coincide between GTAP-Power v12a and the ENTICE-extended database for both production and value added, confirming that the disaggregation adds sectoral granularity while preserving the original sectoral aggregates.

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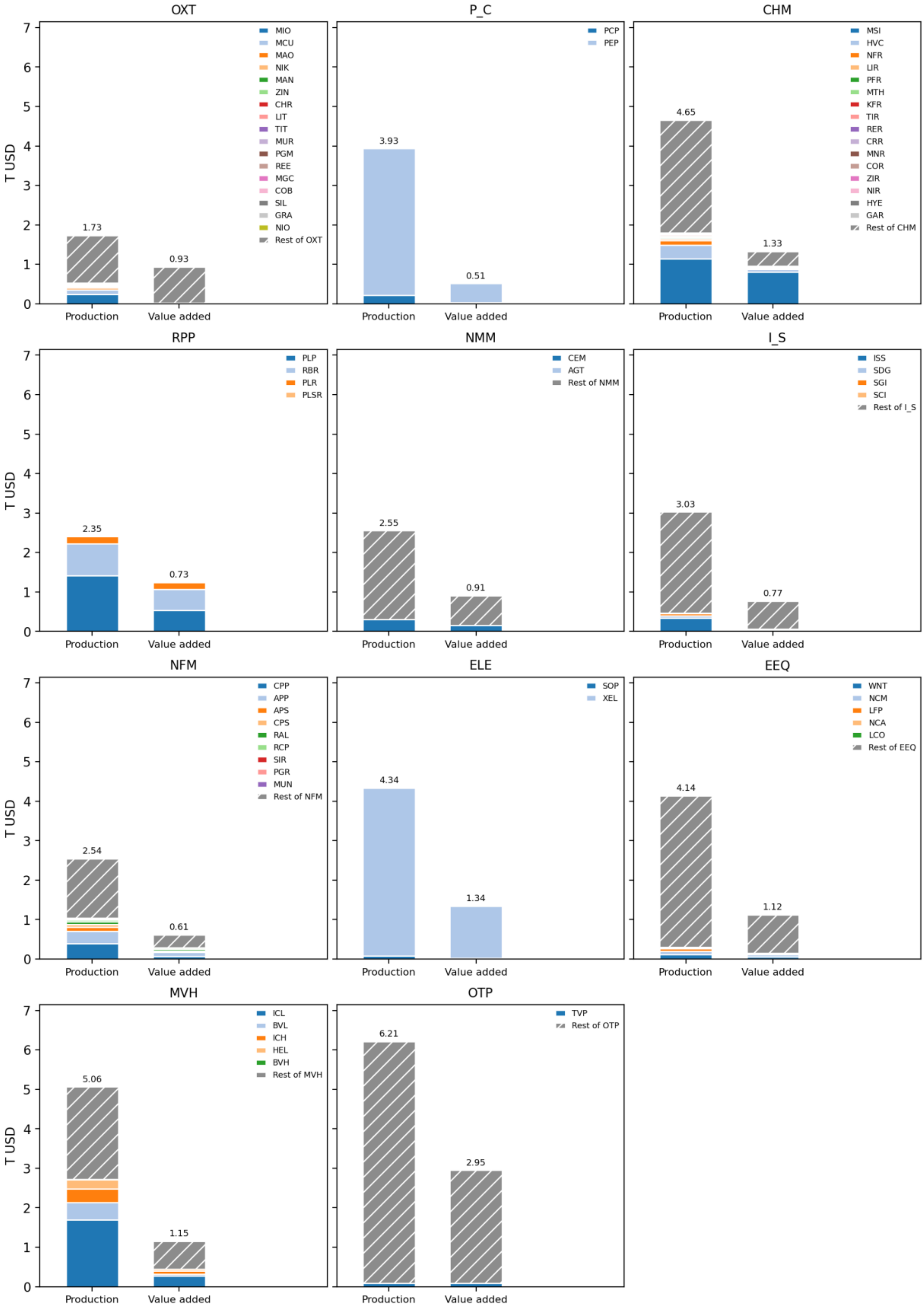

Figure 1. Global production and value added of the original GTAP-Power v12a parent sectors (subplot titles), decomposed into the new ENTICE sectors (legend); "Rest of ..." is the residual parent sector. Values in trillion USD (T USD). Bar totals coincide between GTAP-Power v12a and the ENTICE-extended database, confirming that the disaggregation preserves the original aggregate.

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3 Delivered data

The D2.4 data package provides the sectoral inventories required to extend the GTAP multi-regional input-output (MRIO) database. In line with the GTAP licence conditions, the package does not redistribute a complete extended GTAP database, but it provides the additional sector-level data needed by authorised GTAP users to reproduce the sectoral extension within the MARIO framework (Tahavori et al., 2023).

The delivered inventories are organised as sector-level Excel workbooks. Each workbook describes one new or disaggregated sector to be introduced into the reference database. As the reference database we use the latest version of the GTAP-Power v12a database with 2023 as the reference year. A detailed documentation of the GTAP-Power database is available in Chepeliev (2023) and Peters (2016). The information is provided in a standardized format that can be automatically parsed by the disaggregation software pipeline (i.e. the MARIO-based routine that ingests the sector inventories and applies the disaggregation procedure described in Section 3.4) and used to add the new sector to the parent GTAP sector, while preserving the original aggregate consistency of the database.

These data are intended to be a first release, that will be further expanded in future deliverables, in particular: D2.5 will embed data collection related to agricultural and livestock sectors, D2.6 aims at delivering the transport matrix and D2.8. will provide a fine-tuned comprehensive data release ready to be ingested to the ENTICE GTAP-based models.

Access and dissemination

The current version of the data package is shared with the consortium through the project's internal collaboration space and the I2AM PARIS platform, so that partners can access and review the inventories as they are developed. In line with the project's Data Management Plan (D2.1) and the FAIR principles, public releases are disseminated through open repositories: the disaggregation routine and the guided example are published on GitHub (https://github.com/it-is-me-mario/MRIO-disaggregation-model), while the sector inventories are deposited in the project's Zenodo community with a citable DOI (https://doi.org/10.5281/zenodo.20592035), with explicit links from the project website and I2AM PARIS. Subsequent and final versions - including the inventories added in D2.5 and D2.6 and the consolidated release in D2.8 - will be shared and documented through the same channels, keeping each release traceable from the preliminary D2.4 inventories to the final dataset.

3.1 Delivered file format

Each delivered workbook contains the information required to define the new sector in the MRIO system. The format follows the MARIO add-sector inventory structure and combines metadata, production information, cost-structure coefficients, regional coverage, sector and factor mappings, and trade information where available.

The workbook structure is composed of the following elements:

Table 2. Delivered files description

Excel sheet	Purpose
Summary	Identifies the new sector, the parent GTAP sector and the main sources used
Master	Defines how the inventory is applied in the database extension. Each row links a producing region or regional cluster to the new sector code, the corresponding regional inventory sheet, the parent sector, the unit, and the operation to be performed (Split or Add). The key information is therefore the producing region, the new sector identifier, the name of the inventory sheet to be read, the parent sector, and whether the operation is treated as an addition or a split of the parent sector.
Regional inventory sheets	Provide the input structure of the new sector for each producing region or regional cluster listed in the Master sheet. Each row reports a technical coefficient (input required per unit of sector's output, as indicated in the Master sheet), its unit, the input type (i.e. whether it is an input coming from another sector, or if it is a Factor of production or even a Satellite account), the item code in the database (i.e. name of the sector, factor or satellite account), the region of origin of the input (which can be a cluster), and the operation to apply ("update" means the original coefficient within the database will be updated with the one given in the inventory). The regional inventory sheets are therefore the operational representation of the cost structure used to construct the new sector.
Total outputs	Reports the monetary output of the new sector by region. Each row identifies the sector, the region, the output quantity, and the unit. When direct regional output data are not available, the values reported in this sheet reflect the reconciliation and gap-filling rules described later in the document (Section 3.5).
Trade flows	Reports bilateral trade information for the new sector when sector-specific evidence is available. The sheet identifies the traded sector, the origin region, the destination region, the trade value and the unit. These data are used as trade constraints in the disaggregation only where available; missing trade rows do not imply zero trade unless this is explicitly supported by the source data.
Region clusters	Defines regional aggregates used in the inventory. These clusters allow one inventory or one output value to represent multiple GTAP regions when region-specific data are not available
Sector clusters	Defines groups of input sectors used when the available cost-structure information is more aggregated than the target GTAP sectoral resolution
Factor clusters	Defines groups of value addedvalue-added factors inputs when factor information is available at a more aggregated level than the target factor classification.
Database units	Defines the units used for sectors, factors of production, and satellite accounts in the GTAP database

The regional inventory sheets are the core component of the workbook. Each row represents one input requirement of the new sector. Rows identify the quantity coefficient, the type of input, the database item to be updated, the region of origin of the input, and the type of operation to be applied. Intermediate inputs are reported as sector inputs, while value-added components are reported as factors of production. The coefficients are expressed in monetary terms and are intended to represent the input structure per unit of output of the new sector.

Where the available evidence supports a region-specific cost structure, the workbook contains a dedicated regional inventory. Where data are available only for broader geographical aggregates, the inventory uses regional clusters. These clusters are then expanded to the GTAP regional classification during the database extension procedure. This approach avoids forcing unsupported region-level differentiation while still allowing the new sectors to be represented across the full regional coverage of the model.

The total output table provides the scale of the new sector in each region. These values are required to transform input coefficients into flows and to determine the size of the residual part of the parent sector. Trade information is included when sector-specific bilateral trade data are available. When trade data are not available, the corresponding trade constraint is not imposed, and the disaggregation relies on the other information available for the sector.

3.2 Original data collection, main sources and assumptions

The inventories were built from a coordinated data collection process involving the **T2.2** and **T2.3** contributors, as well as several other consortium partners, involved in other related tasks (**T3.2, T3.3**) contributing sector-specific expertise. This coordination was necessary because several of the new sectors are relevant not only for the GTAP database extension, but also for later modelling work on technologies, mitigation pathways, industrial transformation, and trade-climate interactions.

The original data collection focused on three types of information:

- **Cost structures** of the new sectors, expressed as input coefficients for intermediate inputs and primary factors.
- **Regional total output values**, used to determine the size of the new sector within each parent GTAP sector.
- **Bilateral trade values**, used where available to constrain the geographical allocation of flows for the new sector.

Partner-provided inventories were collected through a common template. The template requested the mapping of each input to the target sector and factor classification, the geographical scope of each inventory, the unit of measurement, the origin of inputs when known, total production values, and the main references used. Additional documentation was collected to describe sector-specific assumptions, data transformations, exclusions, or technology choices.

For a large share of mining, refining, and material-related sectors, the inventories were complemented or constructed using data assembled by past and ongoing efforts of PURDUE colleagues, including various extensions of the GTAP Data Base, such as GTAP Circular Economy (Chepeliev, 2026) and GTAP Critical

Minerals (Chepeliev et al., 2025). In the cases of mining and refining activities, a general approach for estimating values of output for the corresponding sectors was to rely on the mining and refining data from the United States Geological Survey and British Geological Survey databases, while deriving prices from the trade data flows (with available quantity and value flows across countries and commodities). Considering the corresponding extensions have been developed for the GTAP versions 11 with 2017 reference year, for the purposes of the current deliverable corresponding data collections have been updated to match the 2023 reference year of the GTAP version 12 Data Base. These data include sectoral cost structures, total output targets, bilateral trade information, and mapping tables linking the target ENTICE sectors to GTAP, harmonized system (HS) codes, and related other classifications. These sources were used to provide broad regional coverage and to ensure consistency between sector definitions, production values, and trade information.

Additional sources were used depending on the sector. EXIOBASE data (Stadler et al., 2026) were used when they provided a more detailed representation of the relevant production activity than the parent GTAP sector and for the cases, when data from other inventories was not available. CEPII BACI (Gaulier and Zignago, 2010) and ITC MACMAP (ITC, 2026) databases were used to support trade allocation (using the developed ENTICE-to-GTAP concordances at the HS6 levels of commodity detail) and estimate bilateral tariffs. Existing GTAP data were used as the reference aggregate structure, particularly for parent-sector outputs, regional weights, and consistency checks.

The harmonisation of these sources required a common set of assumptions:

- All inventories were converted to the same monetary accounting logic used by the target database.
- Input items were mapped to the GTAP-based sector and factor classification used in ENTICE.
- When source data were more aggregated than the target classification, sector, factor, or regional clusters were used instead of assigning unsupported detail.
- The parent GTAP sector was treated as the accounting envelope within which the new sector is introduced. This means that the new sector and the residual parent sector jointly preserve the original aggregate representation of the database.

The data collection process therefore did not aim to create a standalone sectoral database independent of GTAP. Its purpose was to provide the additional information needed to disaggregate selected GTAP sectors into policy-relevant activities while maintaining compatibility with the original GTAP accounting structure and with the MARIO implementation used in ENTICE.

The construction of the D2.4 inventories follows a common workflow designed to transform heterogeneous sectoral evidence into a consistent set of MARIO-readable inputs for extending the GTAP-based MRIO database. The workflow has three objectives:

1. To express all sectoral evidence in a common input-output accounting format.

2. To ensure that each new sector is linked to a parent GTAP sector and to the relevant regional coverage.

3. To provide the information required to disaggregate the parent sector while preserving the aggregate consistency of the original database.

The workflow distinguishes between the construction of the sector inventories and the subsequent database disaggregation. The inventories describe the new sectors in terms of cost structures, total outputs, regional applicability, and trade information where available. The disaggregation routine then uses these inventories to introduce the new sectors into the MRIO system and to define the corresponding residual part of each parent sector.

3.3 From data collection templates to final inventory

The starting point of the workflow was to assign each new sector a short code, a descriptive name, and parent GTAP sector. The parent sector defines the accounting envelope from which the new sector is extracted: part of an existing GTAP sector is represented as a more detailed activity, and the remaining part is retained as a residual parent sector.

The data collection templates, once filled and revised, have been collected and harmonized in a complex workflow.

Cost structure harmonization

Harmonisation of the cost structures involves checking that each input is mapped to an admissible sector, factor, or satellite account; converting names and labels to the target classification; resolving cases where source categories are more aggregated than the target database; and defining regional applicability. When an input cannot be assigned to a single target sector without adding unsupported detail, it is represented as a sector cluster. The same logic is used for factors of production and regions.

The regional dimension is treated explicitly. A cost structure can be region-specific, cluster-specific, or global. Region-specific inventories are used when the source provides sufficient evidence for a given GTAP region. Cluster-specific inventories are used when evidence is available for a group of countries or a broader geographical aggregate. Global inventories are used as fallback representations when no more detailed regional evidence is available. This structure allows the workflow to preserve the information content of the original source without pretending that region-level detail exists where it does not.

Total outputs harmonization

Total output values are used to scale the unit cost structures. For each new sector and region, the total output determines the size of the new sector within the parent sector. When a total output value is directly available for a GTAP region, it is used as the preferred value. When output information is available only for regional aggregates, it is allocated to member regions according to the reconciliation rules described in Section 3.5. When no direct or cluster-level value is available, an estimate is derived from the observed relation between the new sector and its parent sector in regions where data are available.

Trade flows harmonization

Trade flows are used only when sector-specific bilateral evidence is available. They provide information on the geographical allocation of the new sector's output across destination regions. In the disaggregation model, trade data are treated as constraints on the relevant bilateral flows. Missing trade observations are not interpreted as zero trade unless the source explicitly supports that interpretation. Instead, the model

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relies on the existing database structure, the new sector cost structure, and the total output information.

Once the information has been harmonised, each sector is represented as a MARIO-readable inventory. The inventory contains the metadata, regional inventory sheets, clusters, total outputs, trade flows, and units required to reconstruct the sector in the MRIO framework. The harmonised inventory is not only a record of the original data collection, but also an operational input to the database extension routine.

The database extension proceeds in two conceptual stages. First, the inventories are used to build an initial representation of the new sectors. This stage introduces the new sector labels, applies the cost-structure coefficients, scales them by total output, and constructs initial intermediate input, value-added, satellite, and final-demand entries. Second, when the sector is treated as a split of a parent sector, the new sector is reconciled with the original parent sector. The flows assigned to the new sector are removed from the parent, and the remaining flows define the residual parent sector.

The final inventories delivered in D2.4 are therefore the result of a harmonised workflow. They are structured to be readable by MARIO, but they also document the empirical assumptions used to build each new sector. This makes the data package suitable both as a reproducibility input for authorised users and as a transparent record of the preliminary sectoral extension completed for D2.4.

3.4 Disaggregation methodology

The database disaggregation process is performed adopting the MARIO software, and is divided into two steps: deterministic allocation and optimisation. The first step consists of using cost structure coefficients, exogenously provided, to disaggregate the columns of the new sector. Once the use coefficients for the new sector are computed, the flows are obtained by applying the exogenous total output, and the values for the remaining sector are found as the difference from the parent total. The same holds for value added cells. The obtained flows are used as prior for the constrained cross entropy minimization, which ensures consistency to the original table, balancing and considers new sectors' total outputs and trade flows.

The algorithm requires as input, in addition to the initial database in MRIO format, the total monetary output of the new sectors, their cost structure (intermediate consumption of other sectors and value added) in coefficient form, and volumes of trade for the new sectors between regions. The completeness requirement is flexible: the cost structure can be defined for clusters of sectors and is automatically allocated to the full set of sectors following the distribution of the parent sector. Total output (X) is needed for the optimisation; trade data (T), by contrast, are not required for all regions, as the corresponding constraint is activated only when specific data are available.

3.4.1 Optimization model

The equation (Eq. 1–11) define the optimization model that determines the cells related to the modified sectors while balancing the table and ensuring consistency with the aggregated one. The objective function (Eq.1) measures the cross-entropy distance between the endogenous variables and the initial estimates (from step one) of the use of the modified sectors by the rest of the economy and of value added (Eq. 1). The distance measure being minimized is the CE between target variables and priors (Britz, 2021; Golan et al., 1997; Peters, 2016; Robinson et al., 2001). The constraints ensure coherence with the original table (Eq.

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2-6), balance of the modified rows and columns given the exogenous total output (Eq. 7-8), and respect of exogenous trade information (Eq. 9). Moreover, (Eq.10-11) impose null values for cells that had a null parent and for those specified by the user. In practice, equations (Eq.2-9) are implemented as inequalities with a tolerance gap, which can be differentiated: tighter for the constraints ensuring consistency with the original data (Eq. 2–6), which are considered more reliable, and larger for the exogenous trade and total output constraints (Eq. 7-9).

3.4.1.1

$$\min_{Z,Y,V} \sum_{rf,rt} \left(\sum_{sf,st \in S_N} H(Z,Z^0) + \sum_{sf \in S_S, st \in S_R} H(Z,Z^0) \right) + \sum_{f,st \in S_N, rt} H(V,V^0) \qquad (1)$$

$$s.t. \quad \sum_{sf \in S_{RN}} Z\,\alpha(sf,sf') = Zold \qquad \forall sf' \in S'_P,\ \forall st \in S_S,\ \forall rf \in R,\ \forall rt \in R \qquad (2)$$

$$\sum_{sf \in S_{RN}} \sum_{st \in S_{RN}} Z\,\alpha(sf,sf')\alpha(st,st') = Zold \qquad \forall sf' \in S'_P,\ \forall st' \in S'_P,\ \forall rf \in R,\ \forall rt \in R \qquad (3)$$

$$\sum_{st \in S_{RN}} Z\,\alpha(st,st') = Zold \qquad \forall sf \in S_S,\ \forall st' \in S'_P,\ \forall rf \in R,\ \forall rt \in R \qquad (4)$$

$$\sum_{sf \in S_{RN}} Y\,\alpha(sf,sf') = Yold \qquad \forall sf' \in S'_P,\ \forall c \in C,\ \forall rf \in R,\ \forall rt \in R \qquad (5)$$

$$\sum_{st \in S_{RN}} V\,\alpha(st,st') = Vold \qquad \forall st' \in S'_P,\ \forall f \in F,\ \forall rt \in R \qquad (6)$$

$$\sum_{rt \in R} \left(\sum_{st \in S} Z + \sum_{c \in C} Y \right) = X(sf,rf) \qquad \forall sf \in S_{RN},\ \forall rf \in R \qquad (7)$$

$$\sum_{rf \in R} \left(\sum_{sf \in S} Z + \sum_{f \in F} V \right) = X(st,rt) \qquad \forall st \in S_N,\ \forall rt \in R \qquad (8)$$

$$\sum_{rt \in R} \left[\left(\sum_{st \in S} Z + \sum_{c \in C} Y \right) \beta(rf,rt) \right] = T \qquad \forall sf \in S_N,\ \forall rf \in R \qquad (9)$$

$$M_{use}\,\mathrm{Z} = 0 \qquad \forall sf \in \mathrm{S},\ \forall st \in S_{RN},\ \forall rf \in R,\ \forall rt \in R \qquad (10)$$

$$M_{supply}\,\mathrm{Z} = 0 \qquad \forall sf \in S_{RN},\ \forall st \in S_S,\ \forall rf \in R,\ \forall rt \in R \qquad (11)$$

3.4.1.2 Definition of operators

$$H(x,y) = (x+\epsilon)ln[(x+\epsilon)/(y+\epsilon)]$$
$$\alpha(sf,sf') = 1 \quad if\ \boldsymbol{sf'}\ is\ parent\ of\ \boldsymbol{sf}, \quad else\ 0$$
$$\beta(rf,rt) = 1 \quad if\ \ rf \neq rt, \quad else\ 0$$

3.4.1.3 Definition of sets

S = Sectors (sector from *sf*, sector to *st*)
R = Regions (region from *rf*, region to *rt*)
F = Factors of production
C = Consumption category

S_N = New sectors
S_R = Residual sectors
S'_P = Parent sectors
S_S = Stable sectors
S_{RN} = Parent and new sectors

3.4.2 Implementation example

A practical implementation of the disaggregation routine described above is publicly available on GitHub (https://github.com/it-is-me-mario/MRIO-disaggregation-model), together with the example data and a guided Jupyter notebook. For illustrative purposes, and to comply with the GTAP licence, the reference GTAP-Power database has been aggregated to a reduced, publicly shareable configuration: two regions (EU27 and Rest of the World), four sectors (Primary, Secondary, Tertiary and Energy), one value-added category and one final-demand (consumption) category per region. The example walks through the extraction of a new "Cement" sector from its parent "Secondary" sector, using two input files: the reduced database and the add-sector inventory.

The procedure follows the same steps applied to the full D2.4 inventories:

- A dedicated Python environment is created, and the project-specific version of MARIO is installed.
- The reduced GTAP database is loaded into MARIO as an input–output table in flow format.
- The add-sector inventory is read, loading the cost structure, total output and metadata of the new "Cement" sector in the standardized format described in Section 3.1.
- The new sector is introduced. The routine performs the two-step procedure of Section 3.4 - deterministic allocation of the cost structure followed by the constrained cross-entropy optimisation - splitting "Cement" out of "Secondary" and defining the residual sector "Secondary_rest"; a residue threshold treats cells below 1 USD as zero. The free CLARABEL solver is used in the example, while MOSEK (free academic licence) is recommended for larger problems.
- The extended database can be explored through its components (intersectoral transaction flows, final demand and value added) which now include both "Cement" and the residual "Secondary_rest".
- The extended table is written back to an Excel workbook (to_excel) for inspection or further use.

While the resulting split is not economically meaningful at this level of aggregation, the example reproduces end-to-end the exact routine used to build the D2.4 inventories, allowing authorised GTAP users to replicate the full procedure step by step. Further operations supported by MARIO are documented at https://mario-suite.readthedocs.io.

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3.5 Data reconciliation and gap filling

The data reconciliation step addresses the fact that the inventories combine data from different sources, classifications, geographical resolutions, and accounting conventions. The purpose is not to remove all uncertainty, but to transform the available information into a coherent set of inputs for the disaggregation methodology.

Output values exceeding parent-sector output

The parent GTAP sector defines the maximum accounting envelope for any sector split. Therefore, the output assigned to the new sector in a given region cannot exceed the output of its parent sector in that region. When a source reports a new-sector output larger than the corresponding parent-sector output, the reported value is interpreted as inconsistent with the GTAP accounting boundary.

This rule preserves the aggregate GTAP output and prevents the disaggregation from creating additional production that is not present in the original database. If several new sectors are split from the same parent sector, the same principle applies to the combined output of all new sectors: their total must not exceed the parent-sector output.

Output reported at regional-cluster level

When output data are available for a regional aggregate rather than for individual GTAP regions, the cluster value is distributed across the member regions using the parent-sector output as a weighting variable.

This rule assigns a larger share of the cluster-level new-sector output to regions where the parent sector is larger. It preserves the cluster total while remaining consistent with the spatial distribution of the parent activity in the original database.

If the parent-sector output is zero for all regions in the cluster, the cluster cannot be allocated using parent-output weights. In such cases, the workflow uses a conservative fallback, such as assigning zero output or using equal weights only when there is independent evidence that the new sector is present in the cluster. The preferred option is to avoid creating production in regions where the parent sector has no accounting support.

Missing regional output values

When no direct or cluster-level output value is available for a region, the output is estimated from the observed relation between the new sector and the parent sector in regions with valid data.

The median of this ratio is computed over regions where both the new-sector output and the parent-sector output are available and where the new-sector output does not exceed the parent-sector output.

The median is used instead of the mean because it is less sensitive to outliers and classification mismatches. Regions where the reported new-sector output exceeds the parent-sector output are excluded from the calculation of the median share, since those observations are treated as inconsistent with the parent-sector accounting boundary.

If no valid ratio can be computed, no unsupported positive output is created. In that case, the new-sector output is set to zero or left to be represented only where evidence exists, depending on the sector and the available source information.

Missing or partial cost structures

Cost-structure information is not always available for every region. The workflow applies the most specific available inventory according to the following hierarchy:

1. Region-specific inventory, when available.
2. Regional-cluster inventory, when available.
3. Global or residual inventory, when no more specific evidence exists.
4. Synthetic inventory derived from similar covered regions, when a global fallback is not appropriate and enough regional evidence exists.

When a synthetic inventory is needed, it is constructed as a weighted average of available inventories from regions belonging to the most relevant geographical cluster. Parent-sector output is used as the preferred weight because it reflects the relative size of the activity in the original database. If all relevant parent-sector outputs are zero, equal weights can be used as a fallback, but only for the purpose of defining a cost structure; total output constraints still determine whether the new sector is active in a region.

This hierarchy ensures that region-specific information is preserved where available, while uncovered regions can still be represented without arbitrary manual assignment.

Aggregated inputs and sector clusters

Some source datasets report input requirements at a more aggregated level than the target sectoral classification. For example, a source may report the use of a broad manufacturing category while the target database distinguishes several manufacturing sectors. In these cases, the workflow does not force the input into a single sector. Instead, the input is represented as a sector cluster.

During the database extension, the clustered input is allocated across its member sectors according to the structure of the parent database. This preserves the aggregate input requirement collected from the source while using the original database to distribute it across detailed sectors. The same principle is applied to factor clusters when value-added information is more aggregated than the target factor classification.

Missing trade data

Trade data are included only when sector-specific bilateral information is available and can be mapped consistently to the target sector. Missing bilateral trade data are not treated as zero. Instead, the corresponding trade constraint is omitted. The model then determines the geographical allocation of the relevant flows from the remaining information: the original MRIO structure, the cost structure of the new sector, total outputs, and any available trade observations.

This treatment is important because product-level trade classifications do not always match activity-based sector definitions. In several cases, the trade product may correspond only imperfectly to the production activity being split from the parent GTAP sector. Treating all missing trade observations as zero would therefore introduce artificial restrictions.

Structural zeros and exclusions

Some flows are known to be structurally absent. These can arise from physical impossibility, classification rules, or explicit exclusions reported during data collection. Structural zeros are preserved during the disaggregation. In the optimisation step, these entries are not allowed to become positive merely to satisfy balancing constraints.

Preserving structural zeros is particularly important for new sectors whose production technology has a narrow input base or for sectors where certain inputs are excluded by definition. At the same time, only well-supported exclusions are imposed, because excessive zero restrictions can make the optimisation infeasible or distort the allocation of flows.

Treatment of residual sectors

Residual sectors are not independent empirical sectors. They are accounting constructs derived from the parent sector after the new sector has been introduced. Their role is to ensure that the disaggregated database can be aggregated back to the original GTAP structure.

The residual sector inherits the part of the parent-sector output, inputs, value added, final demand, and trade structure that is not assigned to the new sector. Where the new sector accounts for the full parent output in a region, the residual sector has zero output in that region. Where the new sector accounts for only part of the parent output, the residual sector represents the remaining activity.

This treatment makes it possible to introduce detailed ENTICE sectors while preserving compatibility with the original GTAP-based database and with modelling applications that still require the original aggregate interpretation.

3.6 Quality assurance and limitations

Taken together, these steps produce inventories that are operational for D2.4 and suitable for reconstructing a preliminary extension of the GTAP-based database while keeping the main accounting assumptions explicit, documented, and traceable. In this sense, the workflow already embeds a practical quality-assurance logic: it is designed to ensure that the inventories can be read coherently within the GTAP-based MRIO structure and used consistently by the MARIO disaggregation routine.

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Main consistency checks and limitations

The main checks embedded in the D2.4 workflow concern accounting and structural consistency, verifying that the parent-sector accounting envelope defined in Sections 3.2 and 3.5 is respected - for each new sector, for the combined set of new sectors split from the same parent, and for the corresponding residual sector.

The workflow also checks whether the delivered inventories can be interpreted as input-output cost structures. This means that intermediate inputs, factors of production, and satellite accounts must be mapped to admissible target items or declared clusters; units must be internally coherent; and regional coverage must be made explicit through region-specific, clustered, or global inventories. Trade information, where available, is used only when it can be mapped consistently and treated as a meaningful constraint without imposing unsupported zero flows.

Figure 1 confirms that parent-sector totals are preserved between GTAP-Power v12a and the extended database.

These checks are substantial, but they should not be confused with a full empirical validation of every sectoral estimate. The strength of D2.4 lies in the internal consistency and operational usability of the delivered inventories, not in the claim that each regional output value, cost structure, or trade pattern has already been benchmarked against the best independent evidence available.

Main Limitations of the preliminary release

The scope of the D2.4 release remains preliminary. The package does not yet provide a complete plausibility assessment of each regional output value, cost structure, trade pattern, or satellite-account coefficient. Several limitations therefore remain visible in the current data package.

First, sectoral coverage is still partial and will be extended in later WP2 deliverables. Second, the underlying sources differ in geographical coverage, sectoral detail, valuation, year, and classification logic, so harmonisation reduces but does not eliminate source uncertainty. Third, some sectors are affected by mismatches between activity-based sector definitions and product-based trade statistics, which limits the interpretation of trade constraints and in some cases also affects output estimates.

Additional limitations arise from the need to use regional clusters, synthetic inventories, or transferred cost structures where direct evidence is not available. Some output values are reconciled or estimated rather than directly observed, residual sectors remain accounting constructs rather than empirically collected activities, and satellite-account coefficients or final-demand allocations are only partially validated at this stage. These features do not make the inventories unusable, but they do define the boundary between what D2.4 already guarantees and what still requires further consolidation.

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4 Conclusions and next steps

This deliverable provides the first release of the sectoral inventories required to extend the GTAP-Power v12a database (2023 reference year) with the energy-intensive and related activities prioritised in ENTICE. It delivers harmonised, MARIO-readable inventories that disaggregate 10 parent GTAP sectors into 76 new sectors - spanning the mining and refining of critical minerals, chemicals and fertilizers, plastics and recycling, cement and other non-metallic minerals, primary, secondary and recycled metals, batteries and solar panels - together with the concordances, cost structures, total outputs and, where available, trade flows needed to reproduce the extension. The accompanying open-source routine and guided example (Section 3.4) make the disaggregation procedure transparent and reproducible for authorised GTAP users.

D2.4 should be interpreted as a harmonised and operational intermediate dataset. It is suitable for reconstructing and testing the preliminary ENTICE extension of the GTAP-based database, for documenting the assumptions used in the introduction of new sectors, and for identifying the areas where additional evidence, expert review, or sensitivity analysis is most needed. As discussed in Section 3.6, the strength of the release lies in its internal consistency and operational usability rather than in a full empirical validation of every sectoral estimate.

Next steps

The transition towards the consolidated database (D2.8) builds on this operational foundation. The main lines of work for the next stage are the following:

- Extend the inventories to the sectoral groups addressed in the forthcoming WP2 deliverables, such as agricultural and livestock sectors (D2.5) and transport-related energy and emission accounts (D2.6) and integrate them with the present inventories in the consolidated release (D2.8).
- Compare the regional output values of the new sectors against independent production statistics prioritising the sectors and regions whose output is currently reconciled or estimated rather than directly observed (Section 3.5).
- Cross-check the input coefficients and value-added shares against sector-specific engineering and economic literature and partner expertise, starting from the sectors built on transferred, clustered or synthetic inventories.
- Carry out a systematic plausibility check of the delivered inventories and of the disaggregated tables before the consolidated release, complementing the internal consistency checks already embedded in the D2.4 workflow.
- Record the main revisions from the preliminary D2.4 inventories to the consolidated D2.8 release, and make data and code available through the project's open repositories (GitHub and the project Zenodo community) in line with the project's FAIR data management plan.

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Annex

Supplementary data and information are provided as Excel files available in the project's Zenodo repository (https://doi.org/10.5281/zenodo.20592035).

"New sectors classification.xlsx" file includes the list of the newly disaggregated sectors, their mapping to the GTAP parent sectors, concordances between newly disaggregated sectors and HS6 line trade data codes, as well as NACE-ISIC sectoral classifications.

Data inventories are included in the sector-specific Excel files, which are named according to the newly disaggregated sectoral notations using sectoral code and a brief description, i.e. **"XXX - sectoral description.xlsx"**. For instance, in the case of the artificial graphite, the file with underlying data is named "AGT - Manufacture of artificial graphite.xlsx".

Each data inventory file is similarly structured and consistent with the data input format required by the MARIO disaggregation utility. The file includes "Summary" sheet, which provides overall information about the file, such as code and description for the newly disaggregated sector (e.g., "AGT", Manufacture of artificial graphite), name of the parent GTAP sector (e.g., "NMM", Non-metallic minerals), version of the inventory (e.g. "Y26M05" - May 2026), as well as the list of the key data sources used to compile the inventory for the corresponding sector (e.g. EXIOBASE, GTAP-CE, GTAP-CM). In the latter case, the references might refer to the composite data sources and underlying methodology, which is further used to provide the 2023-consitent inventories developed here. For instance, this is the case, when referring to the GTAP-CE and GTAP-CM data sources, which were both originally developed for the GTAP version 11 Data Base with 2017 reference year.

The "Summary" sheet also includes links to all other pages in the file. In particular, "Master" sheet which provides analytical structure for the inventory, cluster sheets (regions, sectors and factors), which identify relevant definitions of the clustered/grouped categories, sheets with the output and bilateral trade targets, as well as a set of country-specific sheets, which quantify MRIO-specific linkages.

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